Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

RELATIONSHIPS AMONG PARAOXONASE/ARYLESTERASE ENZYME ACTIVITY AND SERUM LIPID INDICES

Mohammad Esmaiel AFZALPOUR[1], Reza GHARAKHANLOU[2]
Abbas Ali GAEINI[3], Ali Seghatol ESLAMI[1]

Birjand University, Birjand, Khorasan Jonubi, Iran
[2]*University of Tarbiat Modares, Tehran, Iran*
[3] *Faculty of Physical Education & Sport Sciences, University of Tehran, Tehran, Iran*

Human serum paraoxonase/arylesterase (PON/ARE) is synthesized by the liver and its role is hydrolysis of organophosphate compounds in mammals and resistance against atherosclerosis. This enzyme has trimodal phenotype distribution including AA (homozygous low activity), AB (heterozygous middle activity), or BB (homozygous high activity). This study aimed to measure the level of paraoxonase and arylesterase activity and determine the relationships among activity of these enzymes and lipid and non-lipid indices in 25 – 50 year-old healthy men.

Fifty healthy men from Tarbiat Modares University volunteered for this research. The relationships among PON/ARE activity and lipid and non-lipid indices were evaluated by Pearson correlation analysis. We used 2-tailed P-values. The $P < 0.05$ probability was accepted as the level of significance.

Mean PON/ARE activity was 89.14±40.62 and 100.15±36.16 U/L respectively. This means that our participants have lower enzyme activity and total of them classified as AA phenotype. There were no significant relationships among PON/ARE activity and demographic characteristics including age, body mass index, waist to hip ratio or blood pressure. In addition, there were no significant relationships among PON and ARE activity and lipid indices (triglyceride, total cholesterol, LDL and HDL). However, LDL /PON ratio showed significant relationship with HDL/LDL ratio ($r = -0.45$, $P < 0.002$), HDL/total cholesterol ratio ($r = -0.37$, $P < 0.01$), total cholesterol concentration ($r = 0.34$, $P < 0.02$), and LDL concentration ($r = 0.46$, $P < 0.001$).

Weak relationship between serum PON/ARE activity and lipid indices along with low PON activity in studied group suggest that PON/ARE enzyme activity is under influence of genetic and racial factors.

Keywords: paraoxonase enzyme, arylesterase enzyme, serum lipid indices, healthy men

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

A SELF-STABILIZING ALGORITHM FOR THE MINIMAL COLOR SUM OF A GRAPH

Tissaoui ANIS

Laboratoire PRISMa, Université Claude Bernard Lyon 1, 69622 Villeurbanne Cedex, France

The chromatic sum of a graph *G* is the minimum sum of colors in a vertex coloring of *G*. This problem has many interests like in networks, where it models the minimization of the total charge of a network. As systems are more and more large and dynamic, the need distributed approaches able to manage automatically them. In this paper we present a self-stabilizing algorithm to determine a minimal sum of colors for a graph. Such a coloring is determined with at most $O(n\Delta^2)$ changes of colors, where Δ is the maximum degree of the graph.

Keywords: parallel algorithm, self-stabilizing algorithm, vertex coloring

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

SPECTROPHOTOMETRIC DETERMINATION OF ACIDITY CONSTANTS OF CALCON IN WATER AND MIXED WATER-ORGANIC SOLVENTS WITH DATAN ANALYSIS PROGRAM

Mohammad Mazloum ARDAKANI[1], Shahram LOTFI[2], Jahanbakhsh GHASEMI[3],
Alahdad SHABABI[2], Mohammad NOROOZI[4]

[1]*Department of Chemistry, Faculty of Science, Yazd University, Yazd, Iran*
[2]*Department of Chemistry, Payame Noor University, Tehran, Iran*
GilaneGharb Universityi, GilaneGharb, Iran
[3]*Department of Chemistry, Faculty of Science, Razi University, Kermanshah, Iran*
[4]*Research Institute of Petroleum Industry,*
Kermanshah Research Center of Oil & Engineering, Kermanshah, Iran

The acid-base properties of calcon (1-(2-hyroxy-naphthylazo)-2-naphtol-4-sulfonic acid) in water and mixed water-organic solvents at 25 °C and an ionic strength of 0.1 M are studied by a multiwavelength spectrophotometric method. The organic solvents used were the amphiprotic (methanol), dipolar aprotic (dimethyl sulfoxide), and low basic aprotic (acetonitrile). To evaluate the *p*H absorbance data, a resolution method based on the combination of soft- and hard-modeling is applied. The acidity constants of all related equilibria are estimated using the whole spectral fitting of the collected data to an established factor analysis model. Data analysis, carried out by the DATAN package that was developed by Kubista group[1,2] and is called a physical constraints approach, provides a unique solution by requiring that the calculating concentrations obey an assumed equilibrium expression. It has been demonstrated by application to the determination of the acidity constants of two and four protolytic forms of fluorescein. The data analysis program DATAN was applied for determination of acidity constants. The corresponding *p*Ka values have been determined in water and mixed water-organic solvents. There are linear relationship between acidity constants and the mole fraction of different solvents in the mixtures. The effect of solvent properties on acid-base behavior is discussed.

1. Kubista M, Sjoback R, Albinsson B (1993) *Anal. Chem.* **65**, 994.
2. de Juan A, Maeder M, Martínez M, Tauler R (2001) *Anal. Chim. Acta* **442**, 337.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

COMPUTING MARKARACTER TABLE AND USCI TABLE OF FINITE GROUPS

Ali Reza ASHRAFI, Modjtaba GHORBANI

Department of Mathematics, University of Kashan, Kashan 87317-51167, Iran

The concept of a table of marks of a finite group G was introduced by William Burnside in the second edition of his classical book *Theory of Groups of Finite Order*. This table characterize the permutation representations of the group G up to isomorphism and in some detail the partially ordered set of all conjugacy classes of subgroups of G. Recently, a Japanese chemist Shinsaku Fujita[1-4] combined this notion with character table of finite groups to introduce the concept of markaracter table of finite groups. He applied this notion to solve some interesting problems in chemistry.

In this paper, we introduce a new computational approach for calculating markaracter table and also USCI table of finite groups. Using this new method the markaracter tables of well known groups used in chemistry are computed.

1. Fujita S (1998) Markaracter Tables and Q-conjugacy Character Tables for Cyclic Groups. An Application to Combinatorial Enumeration, *B. Chem. Soc. Jpn.* **71**, 1587-1596.
2. Fujita S (1998) Maturity of Finite Groups. An Application to Combinatorial Enumeration of Isomers, *B. Chem. Soc. Jpn.* **71**, 2071-2080.
3. Fujita S (1998) Inherent Automorphism and Q-Conjugacy Character Tables of Finite Groups. An Application to Combinatorial Enumeretion of Isomers, *B. Chem. Soc. Jpn.* **71**, 2309-2321.
4. Fujita S (1998) Direct Subduction of Q-Conjugacy Representations to Give Characteristic Monomials for Combinatorial Enumeration, *Theor. Chim. Acta* **99**, 404-410.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

RECENT GRAPH-THEORETICAL INVESTIGATIONS ON POLYCYCLIC AROMATIC HYDROCARBONS

Alexandru T. BALABAN, Milan RANDIĆ

Texas A&M University at Galveston, Galveston, TX 77553, USA

In collaboration with Milan Randić,* a series of papers was published on partitioning among rings of benzenoids their π-electrons forming the double bonds. When a C=C bond is shared by two rings, each ring is assigned one electron, and otherwise the ring gets both electrons. Thus, a numerical equivalent of the Kekulé structure is obtained (only a few cases of such numerical formulas are known when they correspond to more than one Kekulé formula). The value averaged over all Kekulé structures is the π-electron partition for each ring. It reflects the π-electron density and corresponds closely to Clar structures of benzenoids. Moreover, the contribution of rings being assigned from 0 to 6 π-electrons leads to the "ring signature" which discriminates among various types of rings. For catafusenes, a close correlation with the numbers of zeros in the code is found.

A discussion of observations concerning ring signatures will be presented for catafusenes and perifusenes with up to 7 benzenoid rings.

* *Polycyclic Arom. Comp.*, 2004, **24**, 173; *J. Chem. Inf. Comput. Sci.* 2004, **44**, 50; *New J. Chem.* 2004, **28**, 800; *J. Math. Chem.* 2004, **36**, 271; *J. Chem. Inf. Comput. Sci.* 2004, **44**, 1701; *Z. Naturforsch.* 2005, **60a**, 171; *J. Math. Chem.* 2005, **37**, 443; *Polycyclic Arom. Comp.* 2005, **25**, 215; *J. Chem. Inf. Model.* 2006, **46**, 57.

CHEMODESCRIPTORS AND BIODESCRIPTORS: MATHEMATICAL BASIS AND APPLICATIONS

Subhash C. BASAK

Natural Resources Research Institute, University of Minnesota Duluth, 5013 Miller Trunk Highway, Duluth, MN 55811, USA

The last four decades have witnessed significant developments in the quantification of molecular structure using mathematical techniques derived from graph theory, information theory, and chemical topology. Quantitative descriptors derived by these methods have been used in the prediction of property/biomedicinal activity/toxicity as well as quantification of similarity/dissimilarity of molecules. More recently, analogous mathematical methods have been used in the quantification of structures of biological objects like proteomics maps and DNA sequences. This presentation will discuss latest results in this emerging area of chemo-bioinformatics which deals with the characterization of molecules and biomolecules using mathematical formalisms and their applications.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

USE OF ARBITRARY AND TAILORED MOLECULAR SIMILARITY METHODS IN THE ESTIMATION OF PROPERTY/BIOACTIVITY OF CHEMICALS

Subhash C. BASAK, Brian D. GUTE, Ramanathan NATARAJAN, Denise MILLS

Natural Resources Research Institute, University of Minnesota Duluth,
5013 Miller Trunk Highway, Duluth, MN 55811, USA

Traditionally, practitioners in predictive pharmacology and toxicology have relied on experimentally determined physicochemical properties and bioassay data as well as intuitively selected domain-specific structural criteria for the assessment of complex biochemical and toxicological properties of chemicals. For the majority of chemicals, most of the experimental properties prerequisite to their proper evaluation are not available. One solution to this quagmire is the use of quantitative structure-activity relationships (QSARs) based on calculated molecular descriptors, viz., topological, substructural, geometrical, hydrogen bonding, and quantum chemical (both semiempirical and *ab initio*) indices. In cases where the number of chemicals in a particular class is not enough to develop QSAR, quantitative molecular similarity analysis (QMSA) methods can be used for property/bioactivity estimation based on selected structural analogs of the query chemical. We have developed two types of QMSA methods called the arbitrary and tailored similarity techniques based primarily on topological and substructural descriptors. Whereas the former is based a user-defined structure space, the latter uses a subset of descriptors strongly related to the property of interest. The presentation will report on our recent studies on the relative utility of QSAR, arbitrary QMSA, and tailored QMSA methods in predicting property/activity/toxicity of chemicals.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

EYE SAFE LIDAR WITH COMPUTER CONTROL AND ASSISTANCE

Jernej BODLAJ[1], Tomaž PISANSKI[2,3,4], Franc SOLINA[1],
Boris HORVAT[1,3], Igor POBERAJ[2]

[1]*Faculty of Computer & Information Science, University of Ljubljana, Ljubljana, Slovenia*
[2]*Faculty of Mathematics & Physics, University of Ljubljana, Ljubljana, Slovenia*
[3]*Institute of Mathematics, Physics & Mechanics, Ljubljana, Slovenia*
[4]*Primorska Institute of Natural Sciences & Technology, University of Primorska, Koper, Slovenia*

LIDAR (*Light-Imaging Detection and Ranging*) is a device similar to radar, but uses light instead of radio waves. It can be used for detection of impurities in air polluted by pollutant source like international harbor in our application.

(1) The construction of a mobile eye safe LIDAR, powerful enough to obtain air pollution measurements for a moderately large harbor.

(2) To design and program circuits in an embedded system, required to move LIDAR to a desired spatial orientation, with computer vision assistance through a mounted webcam.

(3) To develop computer software for interactive LIDAR control, data acquisition and further processing. This article focuses mainly on the second and the third objective.

Use of standard reflective telescope and semiconductor photodiode as a sensor. Accommodation of commercial multipurpose Nd:YAG pulsed laser with a purpose of eye safety, used as a source of light pulses. Use of Microchip PIC microcontroller (programmed in C), Hitachi compatible display and simple keypad to build embedded system to drive stepper motors (already mounted in telescope stand) for LIDAR positioning. Use of RS-232 protocol for communication purposes. Use of camera calibration algorithms and picture in picture finding algorithms for fine positioning. Use of modern technology, e.g. C#, for developing user friendly interactive graphical user interface. Database is used to store data and few developed interactive user controls to show it.

Functional mobile LIDAR system with interactive computer support, which in addition to the features described above is planned to be installed in a car or trailer as a part of a portable monitoring system. The system is going to be used mostly to acquire various meteorological and air quality data in a harbor and its vicinity in order to determine the sources of air pollution.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

FROM STRUCTURAL CHEMISTRY TO STRUCTURAL BIOLOGY THROUGH INFORMATION SCIENCE STUDY ON COLLAGEN

Sorana D. BOLBOACĂ[1], Lorentz JÄNTSCHI[2]

[1] *"Iuliu Hațieganu" University of Medicine & Pharmacy, 13 Emil Isac, Cluj-Napoca, 400023, Romania*
[2] *Technical University of Cluj-Napoca, 15 Constantin Daicoviciu, Cluj-Napoca, 400020, Romania*

The work propose the integration of knowledge results from the periodicity/cyclical analysis of amino acids from the protein chains of collagen type one and respectively of knowledge results from principal component analysis into mathematical models. The mathematical models developed based on the results obtained through principal component analysis and time series analysis was applied on collagen type one. The properties of amino acids from the composition of collagen type one was further investigated by the use of *Molecular Descriptors Family* approach, an original methodology that proved its abilities in estimation and prediction of properties and activities of biological active compounds. Web implementation integrates results obtained from the study of amino acids and collagen type one through models translation into online applications: knowledge databases of amino acids and collagen type one, mathematical models obtained through analysis of periodicity/cyclical arrangements of amino acids into the structure of collagen type one and principal component analysis applied on collagen type one. Molecular descriptors and models are able to characterize the relationships between structure and properties.

Keywords: amino acid sequences, collagen, structure-activity relationships (SARs)

Research is partly supported by CNCSIS Romania through grant AT93/2007.

Jäntschi L, Bolboacă S (2007) Results from the Use of Molecular Descriptors Family on Structure Property/Activity Relationships, *Int. J. Molec. Sci.* **8**(3), 189-203.
Bolboacă S-D, Jäntschi L (2007) How Good the Characteristic Polynomial Can Be for Correlations?, *Int. J. Molec. Sci.* **8**(4), 335-345.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

GROWTH INHIBITION ACTIVITY ANALYSIS OF TAXOIDS: INTEGRATION OF STRUCTURE INFORMATION

Sorana D. BOLBOACĂ[1], Lorentz JÄNTSCHI[2]

[11] *"Iuliu Haţieganu" University of Medicine & Pharmacy, 13 Emil Isac, Cluj-Napoca, 400023, Romania*
[2] *Technical University of Cluj-Napoca, 15 Constantin Daicoviciu, Cluj-Napoca, 400020, Romania*

A *Molecular Descriptors Family on Sructure-Activity Relationships* (MDF-SAR) study of the growth inhibition activity for a sample thirty-four taxoids was carried out in order to identify the link between compounds structure and their activity. Two multi-varied models, one with two descriptors and other with four descriptors, proved to have estimation and prediction abilities. Analysis of the statistical characteristics demonstrated that the model with four descriptors has greater abilities to estimate and predict compared with the model with two descriptors. The prediction ability of MDF-SAR model with four variables was tested also with leave-many-out methods. The chance correlation of MDF-SAR model with four variables was investigated using random assignment of compounds in leave-one-out and leave-many-out analysis.

Keywords: molecular descriptors family, structure-activity relationship, MDF-SAR, taxoids, growth inhibition activity

REACTION BETWEEN GUANINE AND THE POTENT CARCINOGEN AFLATOXIN B_1

Urban BREN[1], Matevž BREN[2,3]

[1] *National Institute of Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia*
[2] *Institute of Mathematics, Physics & Mechanics, Jadranska 19, SI-1000 Ljubljana, Slovenia*
[3] *Faculty of Organizational Sciences, University of Maribor, Kidričeva 55a,*
SI-4000 Kranj, Slovenia

We report a series of medium high *ab initio* and density functional theory simulations of guanine alkylation by aflatoxin B_1 *exo*-8,9-epoxide. This reaction represents an initial step of carcinogenesis associated with aflatoxin B_1, a potent genotoxic fungal metabolite. Effects of hydration were considered in the framework of the Langevine dipoles solvation model and the solvent reaction field method of Tomasi and coworkers. *In silico* calculated activation free energies are in a good agreement with the experimental value of 15.1 kcal/mol. This agreement presents strong evidence in favour of the validity of the proposed reaction mechanism and points to the applicability of quantum chemical methods to studies of reactions associated with carcinogenesis. In addition, we predict that the preference of aflatoxin B_1 *exo*-8,9-epoxide over the *endo* stereoisomer for the reaction with guanine exists already in the aqueous solution and is only further amplified in the DNA duplex. Finally, through comparison with an analogous reaction between 3a,6a-dihydrofuro[2,3-*b*]furan *exo*-4,5-epoxide and guanine we show that the large planar body of aflatoxin B_1 does not enhance its reactivity and related carcinogenicity. This explains why the planar region of related mycotoxins sterigmatocystin and aflatoxin G_1 could have been evolutionary optimized in a different way.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

THE HIRSHFELD ATOM IN THE MOLECULE CRITICALLY EXAMINED

Patrick BULTINCK[1], Ramon CARBÓ-DORCA[1,2]

[1]*Department of Inorganic & Physical Chemistry, Ghent University, Gent, Belgium*
[2]*Institute of Computational Chemistry, University of Girona, Girona, Spain*

The concept of an atom in a molecule is a very important one in chemistry because molecules are usually considered as a set of atoms held together by chemical bonds. Unfortunately, such an approach barely has a good theoretical basis. Moreover, the lack of a good definition has opened the door to the existence of many different approaches to identifying the atom in the molecule (AIM). Among the AIM definitions currently in use, one of the preferred ones is based on the Hirshfeld method.[1] There, an AIM density function is constructed using a weight function as follows:

$$\rho_A(\mathbf{r}) = w_A(\mathbf{r})\rho(\mathbf{r})$$

Where the weight function is a positive definite one:

$$w_A^H(\mathbf{r}) = \frac{\rho_{A,Z_A}^0(\mathbf{r})}{\sum_{A=1}^{M} \rho_{A,Z_A}^0(\mathbf{r})}$$

A so-called promolecular density function $\rho^0(\mathbf{r}) = \sum_{A=1}^{M} \rho_{A,Z_A}^0(\mathbf{r})$ is constructed by the simple superposition of atomic densities for the atoms arranged in the same way as in the molecule.

All applications of the Hirshfeld-technique up to now rely on the use of neutral atom densities $\rho_{A,Z_A}^0(\mathbf{r})$, that is: atomic densities that integrate to for every atom to the atomic number Z_A. This, however, has long been recognized as a flaw.[2] Moreover, the information entropy background of the Hirshfeld recipe entails that for the proper definition of the AIM, the isolated atom density should have the same population as that for the AIM.[3]

In the present lecture, a new algorithm[4] is introduced where several problems with the Hirshfeld scheme are solved. The so-called iterative or self consistent Hirshfeld-I scheme removes arbitrary decisions, is more in line with information entropy and allows the use of the Hirshfeld scheme for charged systems.

1. Hirshfeld FL (1977) *Theor. Chim. Acta* **44**, 129.
2. Davidson ER, Chakravorty S (1992) *Theor. Chim. Acta* **83**, 319.
3. Parr RG, Ayers PW, Nalewajski RF (2005) *J. Phys. Chem.* A **109**, 3957.
4. Bultinck P, Van Alsenoy C, Ayers PW, Carbó-Dorca R (2007) *J. Chem. Phys.,*in press.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

QSAR, ADME AND STATISTICS

Darko BUTINA

ChemoMine Consultancy Ltd., 201 Icknield Way, Letchworth Garden City, Herts SG6 4TT, UK

There are many instances in the literature when the author(s) make statements like:

- "It is well known fact …"
- "We all know ….."
- "We have demonstrated in this paper that ….."
- "We have computational model with very good predictive power …."

This presentation will address some of those statements and emphasise the importance of checking all the referenced papers to check the validity of the papers in question.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

QUANTUM QUANTITATIVE STRUCTURE-PROPERTIES RELATIONSHIPS (QQSPR)

Ramon CARBÓ-DORCA[1,2], Sofie VAN DAMME[1]

[1]*Department of Inorganic & Physical Chemistry, Ghent University, Krijgslaan 281, (S3) B-9000 Gent, Belgium*
[2]*Institut de Química Computacional, Universitat de Girona, Girona 17071, Catalonia, Spain*

The theoretical basis of *Quantum Quantitative Structure-Properties Relationships* (QQSPR) is discussed. Some relevant mathematical tools are defined firstly. They are composed by the concepts of tagged sets, vector semispaces and convex conditions. These tools are connected with the description of *Quantum Objects* (QO), and their collections: the QO *Sets* (QOS). QO are made of well-defined submicroscopic systems with an attached known density function. A QOS can be divided into two subsets:

(1) the *Core Set* made of QO with a known observable property value with C-QO as elements and

(2) the *Unknown Set* consisting of QO without a known property, constructed by U-QO elements.

The QOS density functions can be employed as the background basis set, allowing building the *QQSPR operators* up. In turn, by using the quantum mechanical expectation value computation concept, the QQSPR operators allow set up the *Fundamental QQSPR Equation* (FQQSPRE), featuring *Quantum Similarity Measures* (QSM) as fundamental building blocks.

Such a theoretical development permits to find quantitative relationships between any kind of QO and complex observable properties.

Such relationships possess the following characteristics:

(1) Provide QO with *universal* descriptors, the QSM matrices, able to be used within any set of submicroscopic systems description.

(2) QSM constitute QO *unbiased* descriptors, independent of the user.

(3) The FQQSPRE permits to consider a *causal connection* associated to the relationship between submicroscopic systems structure and QO observable properties.

(4) Restricted solutions of the FQQSPRE constitute a set of algorithms, which permit to obtain property predictions for complex submicroscopic systems for which no definite application of the correspondence principle can be envisaged.

(5) The connection between QQSPR and classical QSPR procedures becomes clearly described.

Keywords: QSPR, quantum QSPR, tagged sets, quantum objects, quantum QSPR operators, quantum similarity measures, fundamental quantum QSPR equation, prediction of unknown QO properties

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

MOLECULAR-DYNAMICS SIMULATIONS OF ACTINIDE-SERIES METAL CLUSTERS

Salih CINAKLI[1], Mustafa BÖYÜKATA[1], Jadson C. BELCHIOR[2]

[1]*Department of Physics, Bozok University, 66200 Yozgat, Turkey*
[2]*Departamento de Química - ICEx, Universidade Federal de Minas Gerais, Pampulha, (31.270-901) Belo Horizonte, MG, Brazil*

Geometries, energetics, structural stabilities and magic sizes of the actinide-series metal clusters have been investigated for Ac_n, Th_n, Pa_n, U_n, Np_n, Pu_n, and Am_n up to $n = 50$. Molecular dynamics simulations have been performed via a Morse type potential energy function.[1] Previously determined coordinates through following rearrangement collision in fusion process[2] have been used as initial geometries for energy minimization process. The possible stable structures of these clusters have been calculated. In this report, the lower-lying energy configurations of U_n ($n = 2 - 44$) clusters are presented. The clusters prefer to form three-dimensional compact structures. Binding energies, the first and the second finite difference of the total energy are calculated. There are relevant relations between atomic arrangements in the clusters and the magic sizes. For structural analysis, the point groups, radial distributions and interatomic distances of atoms in the clusters with the second finite differences of their mean values are determined. Additionally, density coefficients with the stability values and the moment of inertia of the lowest-energy structures are analyzed as functions of the number of atoms.

This work was supported by Research Fund of Erciyes University (Project Numbers: FBA.06.07 and FBT.06.56), in part by Bozok University in Turkey and by CNPq with FAPEMIG in Brazil.

1. Guo J, Shen J, Chen N (2006) *Chem. Phys.* **324**, 314.
2. Böyükata M (2007) *J. Theor. Comput. Chem.* **6**, 81.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

PROPERTIES OF AROMATICITY INDICES BASED ON THE ONE-ELECTRON DENSITY MATRIX

Jerzy CIOSLOWSKI[1], Eduard MATITO[1], Miquel SOLÀ[2]

[1]*Institute of Physics, University of Szczecin, Wielkopolska 15, 70-451 Szczecin, Poland*
[2]*Institute of Computational Chemistry & Department of Chemistry, University of Girona,*
17071 Girona, Catalonia, Spain

Proper normalization of two previously published indices yields aromaticity measures that, when computed within the HMO approximation, match closely the topological resonance energies per π electron of aromatic annulenes and their ions. The normalized indices, which quantify aromaticity of individual rings in polycyclic systems, are equally applicable to homocyclic and heterocyclic compounds and can be readily computed from 1-matrices calculated at any level of electronic structure theory. However, only the index I_{NG} derived from the Giambiagi formula produces proper ordering of aromaticities of heterocyclic compounds, provided it is calculated from all-electron wavefunctions in conjunction with the AIM partitioning. Its values are shown to be strongly affected by electron correlation effects.

Due to its apparent inability to distinguish between anti- and non-aromatic systems, I_{NG} should be employed only for aromatic species.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

SELECTING THE METHOD FOR A RELIABLE DESCRIPTION OF INTERMOLECULAR POTENTIALS: THE C_{2h}-SYMMETRIC SF_2 DIMER AS A TEST CASE

Jiří CZERNEK

Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic,
Heyrovsky Square 2, 16206 Prague, The Czech Republic

The knowledge of reliable intermolecular potentials is indispensable for quantitative predictions of a variety of properties. *Ab initio* methods of electronic structure theory are capable of providing highly accurate potentials, but the associated computational cost can be huge. Hence, practical schemes for calculation of the interaction energy need to be devised.

This paper concentrates on the model system of a moderate size, i.e., the SF_2 dimer arranged in the way to exhibit the C_{2h} symmetry, and applies a number of quantum chemical techniques to study the dependence of the energy of interaction between the monomers, ΔE, upon the internal coordinate as defined by the distance between sulfur atoms, R. The ΔE values are estimated using both the supermolecule approach (combined with the standard HF, MP2, CCSD, and CCSD(T) models) and perturbation theory (employing the newly developed DF-SAPT-DFT strategy[1]). The family of the X-tuple augmented correlation-consistent polarized-valence basis sets, aug-cc-pVXZ, is adopted and the respective ΔE data are extrapolated to their complete basis set (CBS) limits. In addition, the (3s3p2d2f) set of mid-bond functions[2] is applied together with the aug-cc-pVXZ basis sets to check for an improvement in calculated ΔE values. The resulting $\Delta E(R)$ dependencies are fitted to the same form of the Dunham expansion, and the well depth and the positions of the minimum and of the inflex point are evaluated. The most important finding is a fairly good agreement between an inexpensive DF-SAPT-BVWN/CBS method and the benchmark CCSD(T)/CBS results.

This work has been supported by the Academy of Sciences of the Czech Republic (Project T400500402 in the program "Information Society", Grants IAA400500602 and KJB400500602).

1. Hesselmann A, Jansen G, Schutz M (20005) *J. Chem. Phys.* **122**, Art. No. 014103.
2. Podeszwa R, Bukowski R, Szalewicz K (2006) *J. Phys. Chem. A* **110**, 10345.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

A TOPOLOGY-BASED METHOD FOR CALCULATION OF GROUND-TO-EXCITED STATE CHANGE IN DIPOLE MOMENT

Marina DEKHTYAR[1], Viktor ROZENBAUM[2]

[1]*Institute of Organic Chemistry, National Academy of Sciences of Ukraine, Murmanskaya 5, 02094, Kiev-94, Ukraine*
[2] *Institute of Surface Chemistry, National Academy of Sciences of Ukraine, Generala Naumova 17, 03164, Kiev-164, Ukraine*

A pronounced change in molecular dipole moment on excitation is the necessary prerequisite for a variety of significant physicochemical phenomena, such as solvatochromism, Stark effect, nonlinear optical response, functioning of biological Brownian motors etc. It is thus challenging to screen vast arrays of structures so as to find the promising selections of the molecules remarkable for their outstandingly large ground-to-excited state changes in dipole moment. For this purpose, a sufficiently straightforward topological approach appears appropriate. Accordingly, the working model employed in this study is the long-chain approximation (LCA) of polymethine compounds which represents an analytical approximation of the Hückel molecular orbital method.[1-3] Computationally, it implies manipulation of inverse adjacency matrices raised to different powers.

An analytical expression derived in terms of the topological LCA has been used to estimate ground-to-excited state change in dipole moment for conjugated molecules. The theoretical estimates have been benchmarked against available experimental data and a strong correlation, with $R = 0.982$, has been found between them. The relationship between the molecular topological parameters and the change in dipole moment offers the efficient ways to maximize the latter. Based on the regularities revealed, a large-scale search among more than 1000 heterocyclic residues has been carried out so as to find the structures promising sufficiently large differences in dipole moment between the ground and excited state. As a result, about 50 residues were selected as candidate structures for further stages of the relevant molecular design.

1. Dyadyusha GG, Kachkovskii AD (1975) *Ukr. Khim. Zh.* **41**, 1176. [*Sov. Progr. Chem.***41** (11), 52.].
2. Dyadyusha GG, Ushomirskii MN (1985) *Teoret. Eksperim. Khim.* **21**, 268. [*Theor. Exp. Chem.* **21**, 257.].
3. Dekhtyar ML (1995) *Dyes & Pigments* **28**, 261.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

APPLICATION OF THE NOVEL MOLECULAR ALIGNMENT METHOD USING THE HOPFIELD NEURAL NETWORK TO 3D-QSAR

Kimito FUNATSU, Masamoto ARAKAWA

Department of Chemical System Engineering, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan

Comparative Molecular Field Analysis (CoMFA)[1] has been widely used as a powerful 3D-QSAR (*Quantitative Structure-Activity Relationship*) tool in the field of medicinal chemistry. In CoMFA, the steric and electrostatic field variables are calculated with a probe atom at the intersections of three-dimensional lattice around compound using the Lennard-Jones and Coulomb potentials. Then statistical model is constructed between their field variables and biological activities of molecules. Usually PLS (*Partial Least Squares*) method is used as a regression method. The result of CoMFA can be easily understood by drawing the contour plots of regression coefficients of the PLS model.

CoMFA is frequently used as standard QSAR technique, but some problems still remain. The molecular alignment is one of the key problems in QSAR study. In the CoMFA and most other 3D-QSAR techniques, a proper alignment between molecules is necessary. Since molecular alignment is an important factor in 3D-QSAR analysis, a variety of methodologies have been proposed.[2] We also proposed new method that can solve conformation/alignment problem using 4-way PLS formulation. Possible 3D conformations of all molecules are generated by conformational analysis and they are characterized by field variables of CoMFA with some possible alignment rules. Then 4-way array for 4-way PLS analysis is created according to similarity measure, and conformations largely contributing to inhibitory activity are selected as active conformer by the regression coefficients of 4-way PLS model. To demonstrate the general utility, the data set of glucose analogue inhibitors of glycogen phosphorylase and benzodiazepine analogue inhibitors of cholecystokinin were used as test samples.

Recently, we invested and proposed the novel molecular alignment method with *Hopfield Neural Network* (HNN).[3] This alignment method is based on methodology which solves the pattern-matching problem developed by Doucet et *al*.. The molecules are represented by four kinds of chemical properties (hydrophobic group, hydrogen-bonding acceptor, hydrogen-bonding donor, and hydrogen-bonding donor/acceptor), and then those properties between two molecules are corresponded each other using HNN. In previous paper, 12 pairs of enzyme-inhibitors were used for validation, and our method could successfully reproduce the real molecular alignments obtained from X-ray crystallography. In this paper, we apply the molecular alignment method to three-dimensional quantitative structure-activity relationship (3D-QSAR) analysis. Two data sets (human epidermal growth factor receptor-2 inhibitors and cyclooxygenase-2 inhibitors) were investigated to validate our method. The robust and predictive CoMFA models could be successfully obtained in both data sets.

1. Cramer RD, Patterson DE, Bunce JD (1988) Comparative Molecular Field Analysis (CoMFA) 1. Effect of Shape on Binding of Steroids to Carrier Proteins, *J. Am. Chem. Soc.* **110,** 5959–5967.
2. Arakawa M, Hasegawa K, Funatsu K (2000) Selection of Bioactive Conformations and Alignment Rules by 4-Way PLS Analysis, *J. Comput.-Aided Chem.* **1**, 1-7.
3. Arakawa M, Hasegawa K, Funatsu K (2003) Novel Alignment Method of Small Molecules Using the Hopfield Neural Network, *J. Chem. Inf. Comput. Sci.* **43,** 1390-1395.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

MARVELous WATER

Tibor FURTENBACHER, Attila G. CSÁSZÁR

[1]*Laboratory of Molecular Spectroscopy, Institute of Chemistry, Eötvös University,*
H-1117 Budapest, Pázmány sétány 1/A, Hungary

A new paradigm for high-resolution molecular spectroscopy is introduced. This model Hamiltonian free algorithm inverts the information contained in uniquely assigned experimental rotational-vibrational transitions in order to obtain *Measured Active Rotational-Vibrational Energy Levels* (MARVEL). The procedure starts with collecting, critically evaluating, selecting, and compiling all available measured transitions, including assignments and uncertainties, into a single database. Then, *Spectroscopic Networks* (SN) are determined which contain all interconnecting rotational-vibrational energy levels supported by the grand database of the selected transitions. Adjustment of the uncertainties of the lines is performed next, with the help of robust fitting or worst offender strategies, until a self-consistent set of lines and uncertainties is achieved. Inversion of the transitions through a weighted least-squares-type procedure results in MARVEL energy levels and associated uncertainties. Local sensitivity coefficients can also be computed for each energy level. The resulting set of MARVEL levels is called active as when new experimental measurements become available the same evaluation, adjustment, and inversion procedure should be repeated in order to obtain even more dependable energy levels and uncertainties.

MARVEL has been used to determine energy levels for several isotopologues of water, the most important polyatomic molecule for spectroscopy and the major greenhouse gas. When MARVEL is applied, for example, to the $H_2{}^{17}O$ isotopologue of water, a list of close to 3 000 dependable energy levels, based on more than 8 000 transitions, has been obtained. Work is in progress to treat the more than 100 000 measured transitions of $H_2{}^{16}O$. When MARVEL is used for inverting the information contained in all the pure rotational transitions of several water isotopologues ($H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$, and $D_2{}^{16}O$), an accuracy exceeding that of the A-reduced Watson Hamiltonian is obtained.

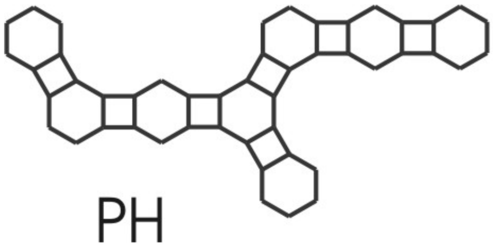
The same procedure can be used for all molecules in order to determine accurate energy levels and eventually as complete molecular spectra as allowed by high-resolution spectroscopic experiments.

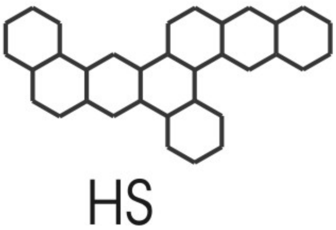
KEKULÉ STRUCTURE BASIS OF PHENYLENES AND THEIR CONGENERS

Boris FURTULA, Ivan GUTMAN

Faculty of Science, University of Kragujevac, P.O. Box 60, 34000 Kragujevac, Serbia

Phenylenes (**PH**) are polycyclic conjugated molecules consisting of 4- and 6-membered rings, in which every 4-membered ring is adjacent to two 6-membered rings, and no two 6-membered rings are adjacent. To every phenylene a benzenoid system, the so-called "*hexagonal squeeze*" (**HS**), can be associated in a natural manner, seen from the below example:





The number of Kekulé structures (*K*) is known to be related to numerous properties of benzenoid molecules. In the case of polycyclic non-benzenoids instead of the Kekulé structure count *K*, the so-called "*Algebraic Structure Soun"t* (*ASC*) plays the analogous role (Dewar & Longuet-Higgins, 1952). In the case of phenylenes, the algebraic structure count is equal to the Kekulé structure count of the corresponding hexagonal squeeze (Gutman, 1993), and in addition *ASC(***PH**) << *K*(**PH**). In view of this, we know *how many* Kekulé structures of a phenylene one has to take into account, but not *which* Kekulé structures.

We now propose a procedure by means of which a subset of Kekulé structures of a **PH** can be selected in a natural and chemically sound manner, the size of which is equal to *ASC*(**PH**) = K(**HS**). Using this Kekulé structure basis, the π-electron structure of phenylenes can be treated in a way fully analogous to the all-Kekulé-structure-based treatment of benzenoid molecules. In particular, we define a Pauling-type bond order, and by means of it calculate the π-electron content of a ring by a procedure analogous to the classical Randić-Balaban approach.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

NON-RIGID GROUP AND SYMMETRY OF TMTB MOLECULE

Modjtaba GHORBANI, Ali Reza ASHRAFI

Department of Mathematics, Faculty of Science, University of Kashan, Kashan, Iran

A molecule is said to be non-rigid if there are several local minima on the potential-energy surface easily surmountable by the molecular system *via* a tunneling rearrangement. A non-rigid molecule typically possesses several potential valleys separated by relatively low energy barriers, and thus exhibits large amplitude tunneling dynamics among various potential minima. Because of this deformability, the non-rigid molecules exhibit some interesting properties of intramolecular dynamics, spectroscopy, dynamical NMR and so all of which can be interpreted resorting to group theory.

In this paper the non-rigid group of TMTB molecule, as well as its topological symmetry are computed.

Keywords: full non-rigid group, TMTB molecule, wreath product

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ON THE ESTRADA INDEX

Ante GRAOVAC

Department of Physical Chemistry, Ruđer Bošković Institute, HR-10002 Zagreb, POB 180, Croatia
&
Faculty of Natural Sciences, Mathematics & Kinesiology, HR-21000 Split, Nikole Tesle 12, Croatia

Some simple estimates of the Estrada index are obtained by applying two theorems from the theory of convex functions.

DELIVERY OF DRUGS BY TAT-TECHNOLOGY

Mira GRDIŠA

Division of Molecular Medicine, Ruđer Bošković Institute, HR-10002 Zagreb, POB 180, Croatia

Peptides derived from a number of proteins are able to enter cells and gain access to the cytosol and nucleus, thus generating much interest in their potential use as vector for intracellular delivery of therapeutic molecules. These peptides have been shown to have potential as cellular delivery vectors for enhancing the activities of their associated cargo, whether they be small molecules such as cytotoxic drugs or macromolecules such as genes and proteins.

TAT technology is a biochemical technique for introduction of full-length peptides or proteins into the cells. This process occurres in a rapid, concentration dependent fashion that appears to be independent of receptors and transporters. It has a broad implication in experimental systems for regulating intracellular processes and has the potential to be use in the development of the new therapeutic strategies for cancer, infectious diseases, and development of vaccines.

TAT transduction system has been exploited and refined to address difficult biological questions. Transduction of TAT-p27 fusion protein clarified cell migration of human HepG2 hepatocellular carcinoma cells. A TAT-p16 fusion protein, a specific inhibitor of cyclin-dependent kinase cdk4/cdk6 complexes, elicited a G1-specific cell-cycle arrest. Also was shown that protein transduced dendritic cells may be effective vaccines for treatment of cancer.

In our hands we have been shown that different forms of TAT-p27 protein can modulate a cell cycle of cultured cell lines, depending on the concentration and type of cells.

Transition of TAT-proteins/peptides use from cell culture systems to animal diseases models has been slow, but the ability of TAT conjugates to protect mice against ischemia, to inhibit tumour growth, and enhance gene delivery, suggests that these offer wide ranging pharmaceutical applications for treating a range of diseases.

SIMPLIFICATIONS OF THE VECTOR INDEX

Ray HEFFERLIN

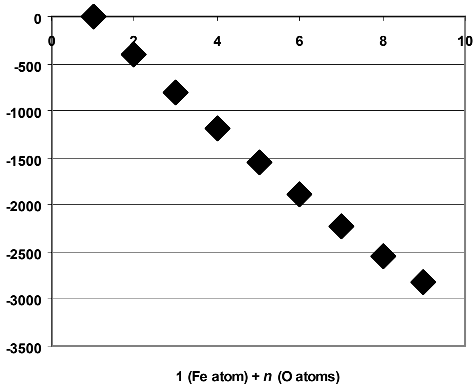
Southern Adventist University, Collegedale, Tennessee37315, USA

The *Periodicity-Sensitive Vector Index for Small Molecules* characterizes a central atom (or molecule) and a progressively larger number (n) of identical atomic (or molecular) ligands or substituents which have some property varying (approximately) linearly with n. The lower component of the index was periodic in the cases investigated.[1] We present a simplification of the method:

- Plot the data on the x axis and n+1 on the y axis.
- Find the least-squares linear fit which passes through $y = 1$ (if the central object is an atom, and the property is the heat of atomization, then x will be zero).
- The upper component of the vector index is the value of the property for the central atom and the lower component is the reciprocal of the slope.

The figure shows $\Delta_a H$ for iron and its oxides in the gas phase[2] after reflection through the line $x = |y|$. The vector index for a series, its property, and its phase was related to the index for any other series, its property, and its phase by matrix multiplication.[1]

We will show that dyadics (or *diagonal* matrices) can simplify the procedure considerably and that they also show periodicity (and second periodicity). The approach is paralleled by that of Zenkevich[3,4] who recently treated the linear dependences of boiling points, refractive indices, dynamic viscosity, surface tension, and several other properties for various series of molecules.



1. Hefferlin R, Luk K (2006) *Croat. Chem. Acta* **79**, 559-571.
2. Latysheva VA, Hefferlin R (2004) *J. Chem. Inf. Comput. Sci.* **44,** 1202-1209 (lower half of Fig. 4.)
3. Zenkevich IG (2006) *Russ. J. Org. Chem.* **42**, 1-11.
4. Zenkevich IG (2006) *Russ. J. Phys. Chem.* **80**, 1636-1642.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

THE CONFIGURATION SPACE OF SMALL UNIT DISTANCE GRAPHS

Boris HORVAT[1], Tomaž PISANSKI[1,2]

[1]*Institute of Mathematics, Physics & Mechanics, Ljubljana, Slovenia*
[2] *Faculty of Mathematics & Physics, University of Ljubljana, Ljubljana, Slovenia*

Graph is a mathematical structure that is sometimes hard to separate from its visualization. An important branch of graph theory studies graph drawing problems. Recently a mathematical approach to graph visualization has been developed under the name of "graph representations".

A graph representation is a mapping from the set of vertices of a graph into some representation space. A unit distance representation of a graph maps adjacent vertices to points at distance 1. A graph with a unit distance Euclidean planar realization is called a *unit distance graph*. In general, a representation may be degenerate in various well-defined senses. Sometimes, only non-degenerate representations, or "realizations" are sought. Another interesting question is to find all distinct degenerate unit distance representations of a given graph.

If the representation space has the structure of a metric space, it is possible to define the energy of a representation. Representations of graphs may exhibit some of the graph symmetry and are usually quite interesting to find. The theory is related to the rigidity theory where linkages are studied. Configuration space of a graph consists of a manifold that can be further factored in order to become an orbifold. Configuration spaces of small unit distance graphs are considered.

Finally, graphs themselves are frequently used for representing other mathematical structures, such as networks, posets, polytopes, maps, tillings, configurations, etc. This, in turn, opens up a possibility of a theory of representations for these structures. In particular, the study of 2- and 3-dimensional unit distance representation of molecular graphs seems to be a topic well suited for the area of mathematical chemistry.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

DEVELOPMENT OF PROTONIC AND DEUTERONIC BASIS FUNCTIONS BASED ON MULTI-COMPONENT MOLECULAR ORBITAL METHOD

Takayoshi ISHIMOTO[1,2], Masanori TACHIKAWA[3], Yuichi INADOMI[4],
Hiroaki UMEDA[1,2], Toshio WATANABE[1,2], Umpei NAGASHIMA[1,2]

[1]*Research Institute for Computational Science, National Institute of Advanced Industrial Science & Technology, Tsukuba, Ibaraki 305-8568, Japan*
[2]*Core Research for Evolutional Science & Technology (CREST), Japan Science & Technology Agency, Kawaguchi, Saitama 332-0012 Japan*
[3]*Quantum Chemistry Division, Graduate School of Science, Yokohama City University, Kanazawa-ku, Yokohama 236-0027, Japan*
[4]*Computing & Communications Center, Kyushu University, Sawara-ku, Fukuoka 814-0001, Japan*

In order to theoretically describe the nuclear quantum effects, several approaches beyond the Born-Oppenheimer approximation have been used. Especially, we proposed the *Multi-Component Molecular Orbital* (MC_MO) method[1] which can take into account the quantum effect of proton/deuteron. In these methods, because both nuclear and electronic molecular orbitals are expressed as linear combination of *Gaussian-Type Functions* (GTF), it is necessary to develop basis functions for the nucleus, which have not yet been systematically determined in terms of GTF exponents and centers. In this study, we analyzed the exponent (α) values in GTF for protons and deuterons in BH_3, CH_4, NH_3, H_2O, HF, and their deuterated molecules for the development of nuclear basis functions[2] (*Table 1*).

The α_{ave} value of optimized α in [1s1p] GTF for proton by MC_MO-MP2 is smaller than the one by MC_MO-HF due to the electron-nucleus correlation effect. Our developed protonic basis functions treat the quantum effects of proton and deuteron effectively and extend the application ranges of the MO calculation to include nuclear quantum effects.

Table 1. Optimized exponent (α_s and α_p) values in [1s] and [1s1p] GTFs for protons in various H-compounds using the 6-31G(*d,p*) electronic basis functions.

H-Compounds			BH_3	CH_4	NH_3	H_2O	HF	α_{ave}
HF	[1s]	α_s	24.2590	24.6317	24.5875	24.1503	23.2838	24.1825
	[1s1p]	α_s	24.2726	24.6270	24.5923	24.1378	23.2906	24.1841
		α_p	23.0000	23.5040	23.5015	22.9924	23.0078	23.2011
MP2	[1s]	α_s	24.3872	24.5263	24.3331	23.8004	22.9689	24.0032
	[1s1p]	α_s	21.0827	21.2506	21.0339	20.2756	19.3130	20.5912
		α_p	22.1053	22.1196	21.8066	21.4476	20.8439	21.6646

1. Tachikawa M (2002) *Chem. Phys. Lett.* **360**, 494.
2. Ishimoto T, Tachikawa M, Nagashima U (2006) *J. Chem. Phys.***125**, 144103.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

AB INITIO FRAGMENT MOLECULAR ORBITAL STUDY OF MOLECULAR INTERACTIONS BETWEEN LIGANDED RETINOID X RECEPTOR AND ITS COACTIVATOR

Mika ITO[1,2], Kaori FUKUZAWA[3], Yuji MOCHIZUKI[2,4],
Tatsuya NAKANO[2,5], Shigenori TANAKA[1,2]

[1]*Graduate School of Human Development & Environment, Kobe University, Kobe, Japan*
[2]*CREST, Japan Science & Technology Agency*
[3]*Mizuho Information & Research Institute, Inc., Tokyo, Japan*
[4]*Department of Chemistry, Faculty of Science, Rikkyo University, Tokyo, Japan*
[5]*Division of Safety Information on Drugs, Food & Chemicals, National Institute of Health Sciences, Tokyo, Japan*

The *ab initio Fragment Molecular Orbital Method* (FMO) calculations were performed for retinoid X receptor (RXR) complex (*Figure 1*) with its ligand 9-cis retinoic acid (9cRA) and steroid receptor co-activating factor-1 (SRC1) to examine the influence of mutations in transcriptional activation function 2 activating domain core (AF2C) of RXR on molecular interactions between 9cRA liganded RXR and SRC1. The RXR–SRC1 interactions in three types of XR-9cRA-SRC1 complexes were compared. A wild type (WT), a mutant whose Glu453 of AF2C was substituted by Lys (E453K), and another mutant whose Glu456 of AF2C was substituted by Lys (E456K). Glu453 is known as a highly conserved charged residue and have important roles as a clamp of SRC1 and an electron donor for SRC1.[1] Through the comparison of WT, E453K, and E456K, possible causes of a marked decrease in the transcriptional activity of RXR due to the mutation of Glu453[2] were discussed. It was quantitatively demonstrated that the strength of the RXR-SRC1 interaction correlates with the degree of the transcriptional activation (WT > E456K > E453K).[2] In E453K, the RXR-SRC1 interaction was extremely impaired by the AF2C–SRC1 repulsive interaction, and the charge transfer from RXR to SRC1 was impaired by the decreased electron donation from RXR to SRC1. Our findings suggest that the inhibitions of the RXR-SRC1 interaction and of the charge transfer from RXR to SRC1 would be the possible causes for the marked decrease in the transcriptional activity of RXR.

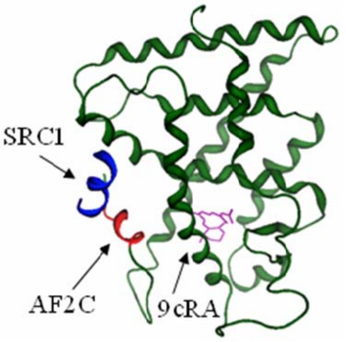


Figure 1. RXR-9cRA-SRC1 complex

1. Ito M, Fukuzawa K, Mochizuki Y, Nakano T, Tanaka S (2007) *J. Phys. Chem. B* **111,** 3525–3533.
2. Thompson PD, et *al*. (2001) *J. Mol. Endocrinol*. **27**, 211–227.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

LINE DISTANCE MATRICES IN BIOINFORMATICS

Gašper JAKLIČ[1], Tomaž PISANSKI[1, 2], Milan RANDIĆ [3]

[1]*IMFM, University of Ljubljana, Ljubljana, Slovenia*
[2]*University of Primorska, Ljubljana, Koper, Slovenia*
[3]*Emeritus at Drake University, Des Moines, Iowa, USA*

In various areas of research sequences of objects have to be studied. In recent years a particular attention was given to biological sequences (study of RNA, DNA and proteins), but sequences appear also in computer science, chemistry, linguistics, ……. The study of similarities among a number of sequences is a hard problem. Instead of direct comparison, one can associate with a sequence a set of invariants, such as a matrix or its eigenvalues. These invariants represent properties of the sequence and can be used as sequence descriptors.

Let $t_1<t_2<\ldots<t_n$ be a given sequence in **R**. Then a *Line Distance Matrix L* is defined with $L_{ij}=|\, t_i- t_j|$. In this paper we are exploring properties of recently introduced Line Distance Matrices, and in particular we consider properties of their eigenvalues. We prove that Line Distance Matrices of size *n* have one positive and *n-1* negative eigenvalues. Visual representation of Cauchy's interlacing property for Line Distance Matrices is considered. Relations with well-known Euclidean Distance Matrices are established.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ANALYSIS OF LIDAR BACKSCATTERING CURVE BY LINE DISTANCE MATRICES

Gašper JAKLIČ[3,4], Klemen BERGANT[7], Jernej BODLAJ[1], Nataša GRLJ[4],
Boris HORVAT[1,3], Peter OGRINC[8], Gorazd POBERAJ[3], Milan RANDIĆ[5,6],
Franc SOLINA[1], Smiljana ŠKVARČ[4], Aleš ZALOŽNIK[3], Marko ZGONIK[2],
Igor POBERAJ[2], Tomaž PISANSKI[2,3,4]

[1]*Faculty of Computer & Information Science, University of Ljubljana, Ljubljana, Slovenia*
[2]*Faculty of Mathematics & Physics, University of Ljubljana, Ljubljana, Slovenia*
[3]*Institute of Mathematics, Physics & Mechanics, Ljubljana, Slovenia*
[4]*Primorska Institute of Natural Sciences & Technology, University of Primorska, Koper, Slovenia*
[5]*National Institute of Chemistry, Ljubljana, Slovenia*
[6]*Drake University, Des Moines, USA*
[7]*Centre for Atmospheric Research, University of Nova Gorica, Nova Gorica, Slovenia*
[8]*Slovenian Forestry Institute, Ljubljana, Slovenia*

Light-Imaging Detection and Ranging (LIDAR) backscattering curve is transformed to a binary sequence which is, in turn amenable to various analyses that were discovered in the area of bioinformatics. The transformation of the signal to the sequence keeps the relevant information about the structure of the signal and enables one to store it in a form of a large integer thus providing a simple means of compact storage of information. A differential analysis of similar curves is indicated and can result in further storage savings. In this paper it is shown how line distance matrix methods can be applied to a collection of similar curves, each of them transformed to a binary sequence.

Keywords: LIDAR, protein sequence, graphical representation, graph, curve transformation, virtual genetic code, line distance matrix, eigenvalues, sequence analysis

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ON OMEGA INDEX OF SOME NANOTUBES

Maryam JALALI, Modjtaba GHORBANI

Department of Mathematics, Faculty of Science, University of Kashan, Kashan, Iran

Let G be the chemical graph of a molecule. The matrix D = [d_{ij}] is called the detour matrix of G, if d_{ij} is the length of longest path between atoms *i* and *j*. In this paper, an exact expression for detour index of some nanotubes, are presented.

Keywords: nanotubes, detour index, chemical graph

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ZAGREB INDICES: EXTENSION TO WEIGHTED GRAPHS REPRESENTING MOLECULES CONTAINING HETEROATOMS

Dušanka JANEŽIČ[1], Ante MILIČEVIĆ[2], Sonja NIKOLIĆ[3],
Nenad TRINAJSTIĆ[3], Damir VUKIČEVIĆ[4]

[1]*National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia*
[2]*Institute for Medical Research & Occupational Health, P. O. Box 291,*
HR-10002 Zagreb, Croatia
[3]*Ruđer Bošković Institute, P.O. Box 180, HR-10002 Zagreb, Croatia*
[4]*Department of Mathematics, University of Split, Nikole Tesle 12, HR-21000, Split, Croatia*

A possible extension of Zagreb indices to weighted graphs representing heterosystems is presented. It is based on the novel definition of the Zagreb indices by a way of the Zagreb matrices. A theorem is given that is valid for the first Zagreb index of strongly weighted graphs.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

GRAPH-THEORETICAL MATRICES IN CHEMISTRY

Dušanka JANEŽIČ[1], Ante MILIČEVIĆ[2], Sonja NIKOLIĆ[3], Nenad TRINAJSTIĆ[3]

[1]*National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia*
[2]*Institute of Medical Research & Occupational Health, P. O .Box 291, HR-10002 Zagreb, Croatia*
[3]*Ruđer Bošković Institute, P.O. Box 180, HR-10002 Zagreb, Croatia*

We will present our book on graph-theoretical matrices in chemistry that appeared earlier this year in the series *Mathematical Chemistry Monographs*, edited by Ivan Gutman and published by the University of Kragujevac. We will also tell the story behind the book.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

COMPUTER SIMULATION OF EVAPORATION AND TRANSPORT OF MULTICOMPONENT MIXTURES IN AIR USING COMSOL MULTIPHYSICS AND COSMOTHERM

Gábor JÁRVÁS, Anett KONDOR, András DALLOS

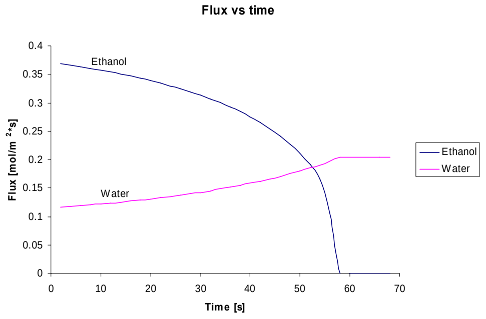
Department of Chemistry, University of Pannonia, Veszprem, Hungary

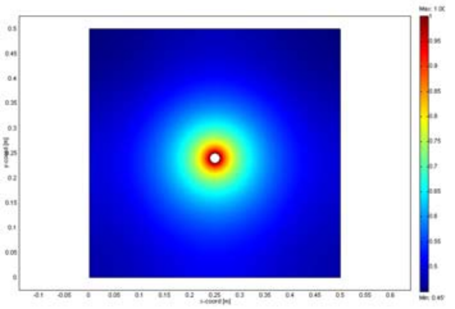
In the absence of convective effects, the evaporation rate of a multi-component system is governed by the rate of diffusion of molecules from the surface. The particle flux at the surface depends on the diffusion coefficient and the concentration gradient of molecules in the gas phase over the surface. The gas phase concentration of the components over the liquid phase is determined by vapor-liquid equilibrium. However, due to the mass lost, the liquid phase composition, the activity coefficients of the components and therefore their concentration and concentration gradients in the gas phase are permanently changing during the evaporation.

The first order unsteady state *evaporation and condensation* of layers and droplets of multi-component mixtures and transport processes of their components were investigated by computer simulation in **MATLAB** environment. The activity coefficients and the vapor pressures of the components were estimated by **COSMOtherm** program, which is based on **COSMO-RS** theory of interacting molecular surface charges computed by quantum chemical methods using **Turbomole**.

The nonsteady state transport of compounds in the gas phase were predicted using a dynamic approach, where the external transfer processes are described by the continuity equation solved by the computer program **COMSOL Multiphysics**. The relation between the molar mass transfer rate, the gas phase concentration gradient and the diffusion coefficient is deduced from the three dimensional nonsteady state version of Fick's law. The Kelvin and cooling effects were taken into account for calculating the evaporation of droplets

The simulations for the permanently changing boundary and initial conditions have resulted in the evaporation flux and spatial concentration profiles of the molecules over the surface and around the droplets, which allowed the estimation of changing in liquid phase composition and the lifetime of the evaporating layers and droplets.





Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

GENERALIZED FOSSE'S METHOD FOR RESOLVING A SUM OF EXPONENTIALS

Željko JERIČEVIĆ

KMS Technologies, Houston, TX 77057, USA
&
Department of Biology & Medical Genetics, Medical School Rijeka, HR-51000 Rijeka, Croatia

$$y = \sum_{i=1}^{N} A_i e^{-k_i t}$$

Exponential decay describes multitude of physical, chemical and biological processes. It is very often the case that the summary signal is measured and individual components have to be extracted by computation. This is a difficult problem because of the non-orthogonality of exponentials and sensitivity to noise.

The method proposed here is from the family of the least squares methods with linearization step based on numerical integration. After the integration, solution of multi-exponential problem is obtained by solving over-determined system of linear equations followed by finding the roots of polynomial equations. The number of exponentials in the signal dictates the degree of polynomial equations, rank of the linear system and multiplicity of numerical integration. This idea was originally suggested by Foss[1] in biostatistics, and also by others in chemistry[2] and biology,[3],but none of the mentioned papers developed the general solution or software for an arbitrary number of exponential terms. The consequence for software development was that only specialized subroutines for each individual case (mono-exponential, bi-exponential, tri-exponential, etc) have been written.

This paper describes development of general solution using Fosse's approximation and opens the possibility of combining signals in a manner of the Global method[4] for achieving superior resolution and improvement in signal/noise ratio. Our modification of the Global method is adapted to linear problem from the original version used in nonlinear regression.

The advantage of accurate linearization with noise cancellation properties is that the exponentials separation becomes fast, non-iterative procedure and condition number of the linear system can be used to monitor the quality of solution. A priori assumptions about the solution are not needed unless used as constrains. The speed and reliability of the method are crucial for processing large data sets in microscopy and NMR imaging where human intervention into optimization process is not feasible and automation of computations is a key.

The summary of major steps in proposed methodology[5] is:

Linearization by numerical integration method

Solution of linear system of equations with or without non-negativity constrains

Determining roots of polynomial equation(s) based on linear system solutions.[6] This step yields non-linear parameters, i.e. decay constants k_i.

Using now known decay constants in order to compute pre-exponential terms A_i.

Testing and verifying the results by detailed error analysis.

1. Foss SD (1970) *Biometrics* **26**, 815-821.
2. Matheson IBC (1987) *Anal. Instr.* **16**, 345-373.
3. Jericevic Z et *al*. (1990) *Adv. Cell Biol.* **3**, 111-151.
4. Knutson JR (1983) et *al.*, *Chem. Phys. Lett.* **102**, 501-507.
5. Jericevic, Z. (2006) USP7088097.
6. Lawson CL, Hanson RJ (1974) *Solving Least Squares Problems*, Prentice-Hall, Englewood Cliffs, p.340.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

EIGENVALUES OF TOROIDAL FULLERENES

Peter E. JOHN, Horst SACHS

Department of Mathematics, Ilmenau Technical University, 98684 Ilmenau, Germany

A *toroidal 6-cage* S is a trivalent graph embedded in (the surface of) a torus all of whose faces are hexagons. Reflecting the structure of (hypothetical) toroidal carbon molecules such graphs are, in a chemical context, also called *toroidal fullerenes*.

In Hückel's model of hydrocarbons (LCAO-MO theory), the eigenvalues of the adjacency matrix of S correspond to the energy levels of the molecule represented by S. Therefore, a simple method that enables these quantities to be determined is required. It is important to note that, by suitable point identification, all toroidal 6-cages can be derived from a common parent, namely, from the regular hexagonal tessellation of the plane (the graphite grid) making use of the twofold periodicity of this structure.

The first, seminal paper on the spectrum of toroidal fullerenes appeared in 1993. Its authors, E.C. Kirby, R.B. Mallion and P. Pollak[1] developed a method (unfortunately, not too simple) that allows the eigenvalues for all toroidal fullerenes with up to 3600 hexagons, and many others, to be calculated.

The second paper on this topic appeared in 2000. A. Ceulemans, L.F. Chibotaru, S.A. Bovin and P.W. Fowler[2] described a general method based on solid-state physics.

Simplifying and generalizing this procedure we shall describe a new method for factoring the characteristic polynomial of any graph of *n*-dimensional toroidal structure derivable from some *n*-dimensional locally finite *n*-fold periodic parent.

1. Kirby EC, MallionRB, Pollak P (1993) Toroidal Polyhexes, *J. Chem .Soc. Faraday Trans.* **89**(12), 1945-1953.
2. Ceulemans A, Chibotaru LF, Bovin SA, Fowler PW (2000) The Electronic Structure of Polyhex Carbon Tori, *J. Chem. Phys.* **112**(9), 4271-4278.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ANALYSIS OF AIR POLLUTANT: SPM AND NO_X AN EXAMPLE OF METROPOLIS OF TOKYO AND CHIBA PREFECTURE, JAPAN

Junko KAMBE[1], Umpei NAGASHIMA[2], Eiko NAKAYAMA[3], Tomoo AOYAMA[4]

[1]*Faculty of Media & Communication, University of Edogawa, 474 Komaki, Nagareyama, Chiba 270-0198, Japan*
[2]*Research Institute for Computational Science, National Institute for Advanced Industrial Science & Technology 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan*
[3]*Faculty of Human Life & Environmental Science, Showa Women's University 1-7 Taishido, Setagaya-ku, Tokyo 154-8533, Japan*
[4]*Faculty of Engineering, University of Miyazaki 1-1 Gakuen-Kibanadai, Miyazaki 889-2192, Japan*

We analyzed air pollution data, suspended particulate matter (SPM) and nitrogen oxide (NO_x) to have an index to efficiently show the pollution level at different locations by using *Principal Component Analysis* (PCA) and *Cluster Analysis* (CA). Air pollution data were measured in 2004 in Metropolis of Tokyo and Chiba prefecture, Japan. In Tokyo, air pollution data for 84 observations points were measured by the Tokyo Metropolitan Government Bureau of Environment. In Chiba, the data for 140 observations points were measured by the Government of Chiba Prefecture. Chiba is located on east of Tokyo.

In monthly average value, NO_x varied widely compared to SPM. No strong correlation between SPM and NO_x has been observed. Observation points were separated into two groups by K-L plot with the first and second principal components of PCA. Observation points in a group had small values of the first principal component and large values of the second principal component. They were located in the second quadrant of the K-L plot. They were mainly located close to a large and crowded road. Another observation points had large values of the first principal component and were located in the first and the fourth quadrant of the plot. They were not close to large road. Monthly variation was large for the first group but small for the second group. November was anomaly in Tokyo and July and November were anomaly in Chiba. By CA, the SPM data in November had a different trend in Tokyo, and July and November had a different trend in Chiba. CA showed almost the same trend with PCA.

Severely polluted observation points in Chiba were located in border of Tokyo though observation points in Chiba were almost less polluted in comparison with Tokyo.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

A FREQUENCY ANALYSIS EVALUATION OF SOME OZONE MONITORING STATIONS

Nenad KEZELE[1], Leo KLASINC[1,2], Sean P. McGLYNN[2],
Matevž POMPE[3], Marjan VEBER[3]

[1] *RuđerBošković Institute, HR-10002 Zagreb, POB 180, Croatia*
[2] *Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana, USA*
[3] *Faculty of Chemistry & Chemical Technology, University of Ljubljana,*
Ljubljana, Slovenia

Tropospheric ozone concentrations exhibit pronounced, characteristic diurnal and seasonal cycles. The cycles are usually well defined. Additional oscillations of the ozone concentrations can also occur. However, they are much smaller in amplitude than the 1-year and 1-day cycles and they can be attributed to anthropogenic influence (e.g., specific meteorological and chemical influences on selected monitoring station, periodic station maintenance activities, etc.). Indeed, the spectral analysis of photochemical pollution data can point up hidden conditions that influence particular monitoring stations. Such an analysis by Fourier transform methods was applied to long-term data from 3 US and 14 European ozone monitoring stations. As expected, strong signals were found for the 1-year and 1-day periods. Some weaker signals associable with anthropogenic activities were also observed. A *Principal Component Analysis* (PCA) was applied to the transformed data sets in order to typify these activities. Among others, 7- and 3.5-day frequencies can be considered to be markers of such anthropogenic influences.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

AFFINE FULLERENE IS COMPLETELY GOLDEN

Zdenka KOLAR-BEGOVIĆ[1], Ružica KOLAR-ŠUPER[2]

[1]*Department of Mathematics, University of Osijek, Gajev trg 6, 31 000 Osijek, Croatia*
[2]*Department of Mathematics, Faculty of Teacher Education, University of Osijek,*
Lorenza Jägera 9, 31 000 Osijek, Croatia

GS-quasigroup (*Golden Section* quasigroup) is a quasigroup which satisfies the identity of idempotency aa=a, and the mutually equivalent identities a(ab·c)·c=b, a·(a·bc)c=b. Let ***C*** be the set of all points of a Euclidean plane. If the groupoid (***C***, ·) is defined so that aa=a for any a in ***C***, and for any two different points a, b in ***C*** we define ab=c if the point b divides the pair a, c in the ratio of golden section, then it can be proved that (***C***, ·) is a GS-quasigroup. In this quasigroup all relations and identities which are valid in a general GS-quasigroup can be geometrically interpreted.

In a general GS-quasigroup the geometrical concept of the parallelogram, GS-trapezoid and some other geometric concepts can be introduced. The geometric concept of an affine regular pentagon can be defined by means of GS-trapezoids and the concept of an affine regular hexagon can be obtained using the parallelograms.

Affine fullerene is an affine image of a fullerene. The concept of affine fullerene will be constructed in a general GS-quasigroup using the statements about relationships between affine regular pentagons and affine regular hexagons. Therefore, the affine fullerene can be obtained only by applying the golden section.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

SYMMETRY AND NUMERICAL SOLUTIONS FOR SYSTEMS OF NON-LINEAR REACTION DIFFUSION EQUATIONS

Sanjeev KUMAR, Ravendra SINGH

Department of Mathematics, Dr. B. R. Ambedkar University, I. B. S. Khandari, Agra-282002, India

Many important applications are available for nonlinear reaction-diffusion equation especially in the area of biology and engineering. Therefore, a mathematical model for Lie symmetry reduction of system of nonlinear reaction-diffusion equations with respect to one-dimensional agebra is carried out in this work. Some classes of analytical and numerical solutions are obtained and expressed using suitable graphs.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

CHIRALITY OF FULLERENES AND NANOTUBES

István LÁSZLÓ

Department of Theoretical Physics, Institute of Physics,
Budapest University of Technology & Economics, H-1521 Budapest, Hungary

A graph-theoretical procedure was proposed for assigning a chirality descriptor to each enantiomer of a chiral polyhedron, polyhedral molecule or graph, independently of any vertex labeling scheme.[1] Model Cartesian coordinates and rotational strengths are obtained using only adjacency information. A generalized HOMO-LUMO rotational strength is used to associate a sign with a Schlegel diagram and the corresponding three-dimensional structure, polyhedron or molecule. The topological sign gives an unambiguous way of communicating the identity of an enantiomer. The method was originally developed for fullerenes. In the present talk it will be generalized for nanotubes as well.

1. Rassat A, László I, Fowler PW (2003) *Chem. Eur. J.* **9**, 644.

GROWTH IN CATACONDENSED BENZENOID GRAPHS

Primož LUKŠIČ[1], Tomaž PISANSKI[1,2]

[1]*Institute of Mathematics, Physics & Mechanics (IMFM), University of Ljubljana,*
Ljubljana, Slovenia
[2]*University of Primorska, Koper, Slovenia*

The generating function of the sequence that represents the number of graph vertices at a given distance from the root is called the spherical growth function of the rooted graph. This mathematical notion is applied to benzenoid graphs that are used in graph theory to represent benzenoid hydrocarbons. The growth function calculation is generalized to graphs that have an arbitrary connected graph in place of each hexagon. In addition, the connection between the growth function of a finite graph and its Wiener index is established.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

LIGHT POLLUTION AND CANCER

Mladen MARTINIS, Vesna MIKUTA-MARTINIS

Theoretical Physics Division, Ruđer Bošković Institute, HR-10002 Zagreb, POB 180, Croatia

The longer and longer exposure to solar UV radiation in the open and to artificial light at home, offices, laboratories, disco and night clubs and in many other places has become an incresing problem of modern society. In this paper we analyse the spectra of various light sources in common use in solaries, homes and industries with an emphasies on the UV component of the spectra and the relative intensity of the light and colour. The bad effect of UV radiations on eyes and skin is well known in medical literature. Howevcr, new laboratory studies showed that night time exposure to artificial light stimulated the growth of human breast cancer by suppressing the levels of a hormone melatonin.

THE CIRCADIAN RHYTHMS OF SOME BODY FUNCTIONS: STATISTICAL APPROACH

Vesna MIKUTA-MARTINIS

Theoretical Physics Division, Ruđer Bošković Institute, HR-10002 Zagreb, POB 180, Croatia

In mammals, physiology and behavior are subject to daily oscillations that are driven by an endogenous clock. In the absence of external time cues this internal clock generates cycles of approximately but not exactly 24 hours – circadian rhythms.

Many important oscillating phenomena in the human body like the blood pressure, temperature and the heart frequency are influenced by circadian rhythm. The haematopoetic and immune systems in all their components are also characterized by multifrequency oscillations with a dominant rhythm of proliferation and cell functions within circadian, circannual and circavital frequency ranges. We have studied the influence of the chronobiologic rhythms on these oscillating phenomena in humans.

In this research we have explored the influence of the circadian rhythm on some very important oscillating parameters like the number and function capability of immunocompetent cells, cell proteins, immunoglobulins (IgA, IgG, IgM), components of complement, hormons (cortisol) as well as the blood pressure and the heart frequency.

The study was performed on the group of 20 young men in the age between 20 and 23 and experimental results were analysed using ANOVA (ANalysis Of VAriance) and some other tests. It was done in the collaboration with the team in Clinical Hospital Dubrava in Zagreb.

Our analysis suggests the significant influence of chronobiologic oscillations on some physiologic, immune and hormonal parameters. It could be very important in the diagnostic as well as in the application of drugs in therapy.

1. Pauly JE (1983) *Am. J. Anat.* **168**, 365– 388.
2. Schibler U, Ripperger JA, Brown SA (2001) *Science* **293**, 437– 438.
3. Mikuta-Martinis V, Matijević-Mašić Lj (2006) in: *INSC 2006*, (Lazzarini I, ed.), SCTPLS, Pewaukee, pp. 53-54.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

A COMPUTATIONAL MODEL FOR FUZZY COLOR NAMING

Ali MOGHANI

Department of Color Physics, Institute for Colorants, Paint & Coating (ICPC), Tehran, Iran

The extraction of high-level color descriptors is an increasingly important problem, as these descriptions often provide link to image content. In computer vision, color naming has been posed as a fuzzy set problem where each color category is modeled by a function that assigns a membership value to any given sample. When combined with image segmentation, color naming can be used to select objects by color, describe the appearance of the image and generate semantic annotations. To assign a color name from the vocabulary to an arbitrary input color, we then design a perceptually based color naming metric.

This paper presents a computational model for color categorization, naming and extraction of color composition. The proposed algorithm follows relevant neurophysiological findings and studies on human color categorization.

Keywords: color naming, fuzzy sets, computational model

1. Benavente R, Vanrell M, Baldrich R (2006) A data set for fuzzy colour naming, *Color Res. Appl.* **31** (1), 46-56.
2. Corsini P, Moghani GA (2001) On the finite semi-join spaces and fuzzy sets, *Pure Math. Appl.* **12** (4), 337-353.
3. Moghani GA, Ashrafi AR, Davvaz B (2004) On the finite join spaces associated to rough sets, *Pure Math. Appl.* **14** (4), 11-22.
4. Yendrikhovskij SN (2000) A computational model of colour categorization, *Color Res. Appl.* **26** (supp.), 235-238.
5. Benavente R, Vanrell M, Balrich R (2004) Estimation of fuzzy sets for computational colour categorization, *Color Res. Appl.* **29**, 342-353.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

DATA SET FOR DISCRETE MODEL IN COLOR CATEGORIZATION

Ali MOGHANI, Soroor NAGHDI

Department of Color Physics, Institute for Colorantss, Paint & Coating (ICPC), Tehran, Iran

The ability to associate labels to colors is very natural for human being. Though, this apparently simple task hides very complex and still unsolved problem, ranging over many different disciplines from neurophysiology to sychology and imaging.

In computer vision, color naming has been posed as a fuzzy set problem where each color category is modeled by a function that assigns a membership value to any given sample. When combined with image segmentation, color naming can be used to select objects by color, describe the appearance of the image and generate semantic annotations.

In this paper, we propose a discrete model for computational color categorization and naming. Each of the 11 basic color categories identified by Berlin and Kay is modeled as a fuzzy set.

Keywords: color categorization, color naming, fuzzy sets, computational model

1.Benavente R, Vanrell M, Balrich R (2004) Estimation of fuzzy sets for computational colour categorization, *Color Res. Appl.* **29**, 342-353.
2. Moghani GA, Ashrafi AR, Davvaz B (2004) On the finite join spaces associated to rough sets, *Pure Math. Appl.* **14**(4), 11-22.
3. Benavente R, Vanrell M, Baldrich R (2006) A data set for fuzzy colour naming, *Color Res. Appl.* **31**(1), 46-56.
4. Yendrikhovskij SN (2000) A computational model of colour categorization, *Color Res. Appl.* **26**(supp.), 235-238.
5. Corsini P, Moghani GA (2001) On the finite semi-join spaces and fuzzy sets, *Pure Math. Appl.* **12**(4), 337-353.

HIGH-SPEED PSEUDO-ORTHOGONALIZATION FOR THE CAR-PARRINELLO METHOD

Umpei NAGASHIMA[1], Takatoshi HIGUCHI [2], Tomoo AOYAMA[3]

[1]*Research Institute for Computational Science, National Institute for Advanced Industrial Science & Technology 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan*
[2]*Science & Technology, Mizuho Information & Research Institute, Inc.,*
2-3 Kanda-Nishikicho, Chiyoda-ku, Tokyo 101-8443, Japan
[3]*Faculty of Engineering, University of Miyazak,i 1-1 Gakuen-Kibanadai, Miyazaki 889-2192, Japan*

We propose a high-speed pseudo-orthonormalization algorithm for Car-Parrinello simulation which is derived from the Schmidt orthonormalization in partial spaces. Ratio of speed-up depends on dimension of the spaces. The precision is affected by the dimension size. By using the pseudo-orthogonalization, we got speed-up ratio of 3.3 times for 100 vectors of dimension 1500. The precision was O(-2) that was estimated by the amplitude of off-diagonal elements, where the vectors are arranged like as a matrix. The orthonormalization is high-speed. However, the precision is insufficient for general purpose.

We discuss two approaches to improve the precision. One is the introduction of a band structure for vectors, and another is the alternative sign random numbers. Ratio of the improved precision is 2.1 and 1.5, respectively. Those improvements require little CPU time.

We included complex-codes of the pseudo-orthogonalization in the SCF part of the Car-Parrinello method. The SCF energy convergence of the Schmidt and Car-Parrinello method is depicted in *Figure 1*. Trend of convergence was almost the same for both methods and no difference between the results of the pseudo- and the Schmidt-orthogonalizations was observed in 8 digits though CPU cost was reduced to almost a half.

Thus, we believe the pseudo-orthogonalization is useful to speed-up the Car-Parrinello method, especially, it is suitable for over 1000 vectors.

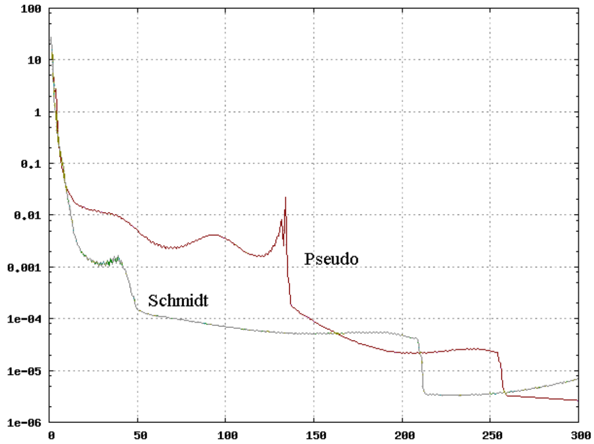


Figure 1. The SCF energy convergence of the Car-Parrinello method.
The vertical axis is the energy [a.u.].
The horizontal axis is the SCF iterations.

NMR SPECTRAL INVARIANTS

Ramanathan NATARAJAN, Subhash C. BASAK

Natural Resources Research Institute, University of Minnesota Duluth,
5013 Miller Trunk Highway, Duluth, MN-55811, USA

Both ^{1}H and ^{13}C NMR chemical shifts were used as QSAR descriptors in predicting biological activities such as binding affinities as well as log$P$. Either the whole spectrum (complete set of chemical shifts) or part of the spectrum (chemical shifts of selected atoms) was used in such studies. We developed a set of NMR spectral invariants by converting ^{1}H-NMR spectra into linear graphs. The approach was extended to diastereomers and enantiomers and for this purpose we used NMR spectra of enantiomeric compounds converted into diastereomers with chiral derivatizing agents. The approach, the challenges and possible solution to the problems will be discussed.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ON THE PATH-ZAGREB MATRICES

Sonja NIKOLIĆ,[1] Nenad TRINAJSTIĆ[1], Damir VUKIČEVIĆ[2]

[1] *Ruđer Bošković Institute, P.O. Box 180, HR-10002 Zagreb, Croatia*
[2] *Department of Mathematics, University of Split, Nikole Tesle 12, HR-21000, Split, Croatia*

The definition of the path-Zagreb matrix for (chemical) trees **PZ** and its generalization to any (molecular) graph is presented. Additionally, the upper bound of $\log_2[PZ(G_{\mathrm{N}})_{ij}]$, where G_{N} is a graph with N vertices is given.

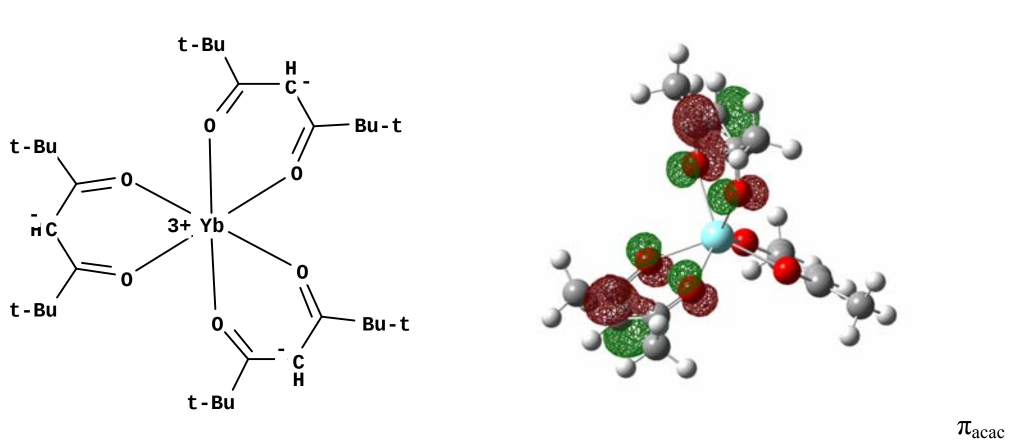
Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ELECTRONIC STRUCTURE OF METAL β-DIKETONATO COMPLEXES

Igor NOVAK[1], Branka KOVAČ[2]

[1]*Charles Sturt University, POB 883, Orange NSW 2800, Australia*
[2]*Physical Chemistry Division, Ruđer Bošković Institute, HR-10002 Zagreb, Croatia*

The electronic structures of yttrium(III), gadolinium(III) and ytterbium(III) tris-2,2,6,6-tetramethyl-3,5-heptanedione (*tmhd*) complexes have been investigated by HeI and HeII uv-photoelectron spectroscopy (UPS), UDFT and OVGF calculations. Metal-ligand bonding in the series of metal β-diketonato complexes is discussed on the basis of empirical arguments. When UPS spectra are measured at several photon energies the changes in relative band intensities provide reliable insight into the nature of valence orbital ionizations. The photoionization cross-sections and orbital energies of metal atoms must both be taken into account in order to rationalize changes in relative band intensities of the HeI/HeII spectra.



Structural formula of Yb(*tmhd*)$_3$ with the coordination sphere of metal resembling a distorted trigonal prism (left) and typical π orbitals in β-diketonato complexes (right)

1. Shibata S, Iijima K, Inuzuka T, Kimura S, Sato T (1986) *J. Mol. Struct.* **144**, 351.
2. Yeh JJ (1993) *Atomic Calculation of Photoionization Cross-Sections and Asymmetry Parameters*, Gordon & Breach, Langhorne.
3. Sansonetti JE, Martin WC (2005) *J. Phys.Chem. Ref. Data* **34**, 1559.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

SOME NEW NUMERICAL CHARACTERIZATIONS OF MODIFIED HAMORI CURVE REPRESENTATION OF DNA SEQUENCES

Igor PESEK[1], Janez ŽEROVNIK[1,2]

[1] *IMFM, Jadranska 19, Ljubljana, Slovenia*
[2] *FS, University of Maribor, Smetanova 17, Slovenia*

The length of DNA sequences makes graphical visualization techniques useful for bioscientists. An advantage of such representations is that they allow visual inspection, helping in recognizing major differences among similar DNA sequences. In recent years, several novel graphical representations of DNA sequences were outlined in the literature and numerical characterizations based on these representations were studied.[2,3]

Numerical characterization of DNA sequences that is based on modified graphical representation proposed by Hamori[1] is considered. While Hamori embeds the sequence into Euclidean space, we use analogous embedding into a cartesian product of graphs, $K_4 \square P_n$, with weighted edges. We set the distance between two consecutive bases (vertices in graphical representation) to be 1 or $\sqrt{2}$ if the two consecutive bases are equal or different, respectively. With these distances we compute a matrix, similar as proposed by Randić,[3] where the off-diagonal entries are given as a quotient of the number of edges between the two vertices and the distance between them. Encouraged by the good results obtained by comparison of products of ten leading eigenvalues,[4] we investigated some other descriptors based on the eigenvalues. For example, we have computed products of first ten and last ten leading eigenvalues and compared them.

The analysis of similarity/dissimilarity among DNA sequences is based on assumption that two DNA sequences are similar if there is very small difference between corresponding products. The results obtained with the new invariants are again very close to the expected behavior showing the robustness of our approach for comparing various DNA sequences. Therefore we conclude that, in spite of its simplicity, the approach proposed gives very promising numerical characterization of DNA sequences.

1. Hamori E (1989) *Biotechniques* **7**(7) 710-720.
2. Randić M, Vračko M, Lerš N, Plavšić D (2003) *Chem. Phys. Lett.* **368**, 583-595.
3. Randić M, Vračko M, Lerš N, Plavšić D (2003) *Chem. Phys. Lett.* **371**, 202-207.
4. Pesek I, Žerovnik J, A numerical characterization of modified Hamori curve representation of DNA sequences, submitted.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

CHEMICAL STRUCTURES FROM THE ANALYSIS OF DOMAIN AVERAGED FERMI HOLES.
PECULIARITIES OF METAL-METAL BONDING

Robert PONEC

Institute of Chemical Process Fundamentals, Czech Academy of Sciences,
Prague 6, Suchdol 2, 165 02, Czech Republic

The nature of metal-metal bonding is analysed and discussed using the recently proposed methodology based on the analysis of the so-called domain averaged Fermi holes. It will be shown that the nature of metal-metal bonding in transition metal chemistry can be often quite peculiar and in many cases its classification exceeds the limits of traditional bonding paradigms exemplified, above all, by the Lewis model of chemical bond as shared electron pair. The richness of metal-metal bonding interactions will be demonstrated on the detailed analysis of the nature of W-W, Fe-Fe, Re-Re and Ga-Ga bond.

1. Ponec R (1997) *J. Math. Chem*. **21**, 323-333.
2. Ponec R, Duben AJ (1999) *J. Comp. Chem.* **8**, 760.
3. Ponec R, Yuzhakov G, Carbo-Dorca R (2003) *J. Comp. Chem.* **24**, 1829.
4. Ponec R, Yuzhakov G, Sundberg M (2005) *J. Comp. Chem.* **26**, 447.
5. Ponec R ,Yuzhakov G, Gironés X, Frenking G (2004) *Organometallics* **23**, 1790.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

A SURVEY OF SODIUM AND POTASSIUM ALTERATIONS DURING REST TIME AFTER AEROBIC ACTIVITIES IN ATHLETES

Mohammad Javad POURVAGHAR[1], Rahman SOORI[2]

[1]*Department of Physical Education, University of Kashan, Kashan, Iran*
[2]*Department of Physical Education, University of Tehran, Tehran, Iran*

The aim of this research has been the investigation of student athletes rest time sodium and potassium variations. For this purpose, 14 students were chosen to take part in this research project. The means and standard deviations of their height, weight, age and body mass index (BMI) were respectively: (175±5.9), (68.27±9.89), (19.56±1.16), (22.08±2.47). Participants trained with incremental continuous running program for 16 sessions with certain and pre-adjusted heart rate intensity and distance. Heart rate intensity was controlled by polar clock. Blood samples were taken from subjects in pre- and post-test in rest condition. Test of running-jugging were performed for determining maximal oxygen consumption (Vo_2 max) of subjects. The analysis of data by SPSS software and paired-sample *t*-test showed that the level of serum sodium was significant after even 24 hours of rest ($P = 0.006$). That may be related to loss of water and fluids of body in the last sessions of training. Also serum potassium level came to its base state in post-test and was not significant ($P = 0.16$). That has been probably for return of extra cellular potassium to intracellular. Mean while, Vo_2 max of subjects was significant after 16 sessions ($P = 0.0001$).

Keywords: sodium, potassium, running-jugging test, aerobic activity

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

CALCULATING THE ESTRADA INDEX

Slavko RADENKOVIĆ, Ivan GUTMAN

Faculty of Science, University of Kragujevac, P.O. Box 60,34000 Kragujevac, Serbia

The Estrada index is a molecular-structure descriptor introduced few years ago by Ernesto Estrada. We denote it by *EE(G)*, where *G* is the underlying molecular graph. The Estrada index is defined as follows.

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the (molecular) graph *G*, i.e., the eigenvalues of the adjacency matrix of *G*. Then

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$$

Thus, for the calculation of *EE(G)* it is necessary to know the spectrum of the graph *G.* Our aim was to design approximate expressions for *EE* that would enable the (approximate) calculation of *EE* knowing only some simple structural features of the underlying graph. In particular, we are interested in *(n,m)*-type approximate expressions, in which the only two graph parameters are *n* = the number of vertices, and *m* = the number of edges.

We found two *(n,m)*-type expressions that in an excellent manner reproduce the Estrada index of benzenoid hydrocarbons:

$$1.098 \cosh\sqrt{\frac{2m}{n}} - 0.64$$ with correlation coefficient 0.99994[1]

and

$$0.979 \cdot \frac{n}{2} \frac{e^x - e^{-x}}{x} - 0.210 \;\; ; \;\; x = \sqrt{\frac{6m}{n}}$$ with correlation coefficient 0.999993[2]

1. Gutman I, Radenković S (2007) *Z. Naturforsch.* **62a,** in press.
2. Gutman I, Graovac A, Radenković S, to be published.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

CANONICAL CODES

Milan RANDIĆ

National Institute of Chemistry, Ljubljana, Hajdrihova 19, Slovenia

We will outline construction of novel type of codes for graphs which encode not only connectivity of a graph but also the canonical labels for vertices. To the best of my knowledge this is the first time that codes were proposed that can allow not only reconstruction of a graph but also reconstruction of accompanying labels for its vertices. The canonical labels used here are obtained by assigning labels to the vertices of graphs so that the rows of the adjacency matrix, when read from the left to the right and from the top to the bottom, produce the smallest binary numbers possible. The canonical codes satisfy all the known requirements for codes: permit lexicographical ordering, being unique, permitting retrieval of the graph, are simple (allowing coding without a recourse to a computer), decoding being simple, there being an effective algorithm for coding, are brief, pronounceable and comprehensible to chemists. In addition the canonical codes are general. They apply equally to trees as well as polycyclic graphs, which is not the case for a number of existing codes for molecular graphs. In the construction of the canonical codes brevity was achieved by eliminating encoding of all "non-essential" zeros of the canonical adjacency matrix. For illustration we present here one of the canonical codes for adamantane, polycyclic $C_{10}H_{16}$, which was first time synthesized in Zagreb in 1941 by V. Prelog and R. Seiwerth. The canonical code of adamantane is given by the sequence: (3, 05, 3, 013, 5, 3, 0007, 0029, 021, 13). Generalization of one of presented novel canonical codes leads to relatively short codes for any adjacency matrix of a graph, whether it is based on the canonical labels for vertices or not. The novel canonical codes will be illustrated on a selection of molecular graphs, graphs representing degenerate rearrangements, and a selection of more general graphs.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ON ^{13}C CHEMICAL SHIFT SUMS IN NONANES

Milan RANDIĆ[1], Marjana NOVIČ[1], Dražen VIKIĆ-TOPIĆ[2], Dejan PLAVŠIĆ[2]

[1]*National Institute of Chemistry, P.O. Box 3430, SI-1001 Ljubljana, Slovenia*
[2]*NMR Center, Ruđer Bošković Institute, P.O.Box 180, HR-10002 Zagreb, Croatia*

^{13}C chemical shifts in alkanes have been studied in the past by linear regression analysis and neural networks, which resulted in acceptable additivity models. We draw attention of NMR spectroscopists to the potential of the partial ordering as a tool for interpretations of selected experimental data. We have examined regularities in ^{13}C chemical shift sum in nonane isomers when viewed as a molecular property and have found that partial ordering provides a better understanding of variations in the relative magnitudes of ^{13}C chemical shift sum in alkanes.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

OVERLAPPING SPHERES VOLUMES AND APICAL COORDINATION

Nenad RAOS[1], Nenad JUDAŠ[2], Ante MILIČEVIĆ[1]

[1]*Institute for Medical Research & Occupational Health, Ksaverska c. 2, POB 291,*
HR-10001 Zagreb, Croatia
[2]*Department for General & Inorganic Chemistry, Faculty of Science, Horvatovac 102a,*
HR-10001 Zagreb, Croatia

The method of *Overlapping Spheres* (OS) was applied for an analysis of coordination of water, carbonyl group, DMSO, and chloride to the apical position(s) of coordination polyhedron of copper(II) chelates with α-amino acids. Altogether 16 crystal structures of copper(II) complexes with glycine, alanine, isoleucine, phenylalanine, threonine, ornithine and 2-aminobutyric acid, along with the copper(II) complexes with 1-amino-1-cyclopropane carboxylic acid were subjected to three kinds of the OS volume calculations.

The fist calculations were performed by placing the central sphere with radius $R_v = 2.5$ Å apically, at the same distance from the copper atom. The second set of calculations were performed by placing the central sphere ($R_v = 2.5$ Å) at the copper atom and separately calculating the OS volumes at both sides of the approximate plane of chelate rings. The third calculations were performed by placing the central spheres apically at "infinite" distance (*i.e.* 400 Å) from copper atom and attributing it $R_v = 400$ Å. In this way for every kind of calculation two OS volumes (V^*) were calculated for each crystal structure, V_A^* and V_B^* ($V_A^* > V_B^*$).

For the first model, in which central sphere was placed apically, linear dependence of V_A^*/V_B^* *vs.* V_B^* was observed ($N = 15$, $r = 0.943$) with a negative slope ($a = -0.304(30)$). The only complex with no apical coordination, bis-(D,L-2-aminobutyrato)copper(II), has the highest V_B^* and estimated $V_A^*/V_B^* < 1$ ($V_A^*/V_B^*{}_{\text{est}} = 0.46$).

The other two models were used for correlation of apical distance, Cu-O$^{\text{ap}}$, *vs.* V_A^*/V_B^*. In both case a function of the form $y = c + b/(a - x)$, with Cu-O$^{\text{ap}}$ assimptote close to 2.3 Å and V_A^*/V_B^* assimptote close to 1 was obtained. The above mentioned compound with no apical coordination found its place on the V_A^*/V_B^* assimptote.

All these results promise that this specific application of the OS method should lead to the models suitable for prediction of the mode of apical coordination.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

TOPOLOGICAL RELATIONS OF THE CHEMICAL ELEMENTS

Guillermo RESTREPO[1,2], Héber MESA[3], Eugenio J. LLANOS[4]

[1]*Laboratorio de Química Teórica, Universidad de Pamplona, Pamplona, Colombia*
[2]*Environmental Chemistry & Ecotoxicology, University of Bayreuth, Bayreuth, Germany*
[3]*Departamento de Matemáticas, Universidad del Valle, Cali, Colombia*
[4]*Corporación SCIO, Carrera 13 N. 13 - 24 oficina 721, Bogotá, Colombia*

We have shown that the chemical groups on the periodic table can be interpreted as similarity neighbourhoods of the properties characterising the chemical elements.[1] In the process of finding these results a new mathematical method combining cluster analysis and topology was developed and nowadays is called "chemotopology".[2] Chemotopology applies cluster analysis to a set whose elements are characterised by different properties. The clusters resulting are regarded as similarity neighbourhoods that become open sets of a topological basis, which makes possible to calculate various topological properties of subsets of interest from the original set. By the application of this method to the chemical elements it was shown that the set of semimetals is the topological boundary of the set of non-metals.[1] The bridge between the cluster analysis results and the topological concepts is set up by the cluster selection on the dendrogram resulting from the cluster analysis. This selection is carried out by cutting the subtrees on the dendrogram containing n or less than n elements. Thereby, the topological basis, and the cardinality of its open sets depend on the selected n.

We showed that the similarity of the elements in the original set can be stressed by considering no disjoint neighbourhoods,[3] as is the case when selecting a particular n. The selection of no disjoint neighbourhoods permits studying in detail the topological relations among different elements of the original set. Here the application of the method to a set of 72 chemical elements characterised by 90 properties (physico-chemical, geochemical and chemical ones) is shown. We calculated five topological properties, namely closures, derived sets, boundaries, interiors and exteriors of several subsets of chemical elements. Finally, a contrast among these results and those obtained by the chemotopological procedure depending on n is made.

1. Restrepo G, Llanos EJ, Mesa HJ (2006) *Math. Chem*. **39**, 401-416.
2. Restrepo G, Villaveces JL (2005) *Croat. Chem. Acta* **78**, 275-281.
3. Mesa H, Restrepo G (2007) *J. Math. Chem*., submitted.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

QSTR WITH EXTENDED TOPOCHEMICAL ATOM (ETA) INDICES. COMPARATIVE QSAR FOR THE TOXICITY OF DIVERSE FUNCTIONAL ORGANIC COMPOUNDS TO *CHLORELLA VULGARIS* USING CHEMOMETRIC TOOLS

Kunal ROY, Gopinath GHOSH

Drug Theoretics & Cheminformatics Laboratory,
Division of Medicinal & Pharmaceutical Chemistry,
Department of Pharmaceutical Technology, Jadavpur University, Kolkata 700032, India

Quantitative Structure-Toxicity Relationship (QSTR) studies on toxicity of 91 organic compounds to *Chlorella vulgaris* have been performed using *Extended Topochemical Atom* (ETA) indices using different statistical tools like stepwise regression analysis, *Multiple Linear Regression with Factor Analysis* (FA-MLR) as the preprocessing step, *Partial Least Squares* (PLS) regression and *Principal Component Regression Analysis* (PCRA). The ETA models have been compared with the non-ETA ones derived from different topological and physicochemical parameters The results show that the QSTR models using ETA descriptors (FA-MLR: Q^2=0.832, PLS: Q^2=0.891, stepwise: Q^2=0.867, PCRA: Q^2=0.741) are comparable to the non-ETA models (FA-MLR: Q^2=0.794, PLS: Q^2=0.897, stepwise: Q^2=0.907, PCRA: Q^2=0.772). Improved results are obtained (except in case of PCRA) when we considered ETA and non-ETA descriptors in combination (FA-MLR: Q^2=0.850, PLS: Q^2=0.913, stepwise: Q^2=0.909, PCRA: Q^2=0.671). The best two models are obtained using combined ETA and non-ETA descriptors applying stepwise regression [Q^2 = 0.909] and PLS [Q^2 = 0.913] techniques. The statistical quality of the best models is better than that of the previously published models. The results suggest that the ETA descriptors are sufficiently rich in chemical information and have ability to encode the structural features contributing significantly to the toxicity of organic chemicals to *Chlorella vulgaris.*

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

Y-RANDOMIZATION AND ITS VARIANTS IN QSPR/QSAR

Christoph RÜCKER[1], Gerta RÜCKER[2], Markus MERINGER[3]

[1] *Biozentrum, University of Basel, Switzerland*
[2] *Institute of Medical Biometry & Medical Informatics, University of Freiburg, Germany*
[3] *Department of Medicinal Chemistry, Kiadis B.V., Groningen, The Netherlands*

Y-randomization is a tool used in validation of QSPR/QSAR models, whereby the performance of the original model in data description (r^2) is compared to that of models built for permuted (randomly shuffled) response, based on the original descriptor pool and the original model building procedure. We compared y-randomization and several variants thereof, using original response, permuted response, or random number pseudo-response and original descriptors or random number pseudodescriptors, in the typical setting of *Multilinear Regression* (MLR) with descriptor selection. For each combination of number of observations (compounds), number of descriptors in the final model, and number of descriptors in the pool to select from, computer experiments using the same descriptor selection method result in two different mean highest random r^2 values. A lower one is produced by y-randomization or a variant likewise based on the original descriptors, while a higher one is obtained from variants that use random number pseudodescriptors. The difference is due to the intercorrelation of real descriptors in the pool. We propose to compare an original model's r^2 to both of these whenever possible. The meaning of the three possible outcomes of such a double test is discussed. The test was applied to several recently published MLR QSAR equations, and cases of failure were identified.

Some progress also is reported towards the goal of obtaining the mean highest r^2 of random pseudomodels by calculation rather than by tedious multiple simulations on random number variables.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

WHY DOES ELECTRON SHARING LEAD TO COVALENT BONDING? A VARIATIONAL ANALYSIS

Klaus RUEDENBERG, Michael W. SCHMIDT

Department of Chemistry & Ames Laboratory USDOE, Iowa State University, Ames, Iowa, USA

Groundstate energy differences between related systems can be elucidated by a *comparative variational analysis of the energy functional*, in which the concepts of *variational kinetic pressure and variational electrostatic potential pull* are found useful. This approach is applied to the formation of the bond in the hydrogen molecule ion. A highly accurate wavefunction is shown to be the superposition of two quasi-atomic orbitals, each of which consists to 94% of the respective atomic 1s orbital, the remaining 6% deformation being 73% spherical and 27% non-spherical in character. The spherical deformation can be recovered to 99.9% by scaling the 1s orbital. These results quantify the conceptual metamorphosis of the free-atom wavefunction into the molecular wavefunction by orbital sharing, orbital contraction, and orbital polarization. Starting with the 1s orbital on one atom as the initial trial function, the value of the energy functional of the molecule is stepwise lowered along several sequences of wavefunction modifications, whose energies monotonically decrease to the groundstate energy of H_2^+. The contributions of sharing, contraction and polarization to the overall lowering of the energy functional and their kinetic and potential components exhibit a consistent pattern that can be related to the wavefunction changes on the basis of physical reasoning, including the virial theorem. It is found that *orbital sharing lowers the variational kinetic energy pressure and that this is the essential cause of covalent bonding in this molecule*.

Work supported by the Division of Chemical Sciences, Office of Basic Energy Sciences, U.S. Department of Energy under Contract No. W-7405-Eng-82 with Iowa State University through the Ames Laboratory.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

PREDICTION OF THE NUMBER OF CARBON ATOMS IN DIFFERENT NANOSTRUCTURES BY USING GEOMETRICAL APPROACH

Hosein SABAGHIAN[1], Gholam Reza VAKILI-NEZHAAD[2], Mehdi VAHIDIPOUR[1]

[1]*Department of Computer Engineering, University of Kashan, Kashan, Iran.*
[2]*Department of Chemical Engineering, University of Kashan, Kashan, Iran*

With growth of nanotechnology, wide ranges of research about chemical and physical properties of nanostructures are performed. Due to relation between physical properties and geometrical structure, understanding of geometrical structure is important. On the other hand, this can be useful for finding unknown structures that have not been produced in laboratory yet.

In this paper, we have studied firstly nanostructures from geometrical point of view. Then an algorithm is proposed for discovering the number of carbon atoms in different nanotubes and fullerenes. In our algorithm, a nanosheet in 2D space is taken as a starting point. Creating 12 nanocones in a nanosheet makes a nanostructure. Different nanostructures are produced by relocation of nanocones.

The result shows that the number of carbon atoms in different nanostructures is a sequence that has infinite harmonies and follows a simple formula. Each harmony is an arithmetic progressive sequence.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

SOME PSYCHOPHYSICAL EXPERIMENTS AND SIMULATION IN COLOR CATEGORIZATION

Mehrdad SAMET, Ali MOGHANI

Department of Color Physics, Institute for Colorants, Paint & Coating (ICPC), Tehran, Iran

Human perceives color in categories, which may be identified using color name such as red, blue, *etc*. The categorization is unique for each human being.

However despite the individual differences, the categorization is shared among members in society. This allows communication among them, especially when using color name. Sociable robot, to live coexist with human and become part of human society, must also have the shared color categorization, which can be achieved through learning. Many works have been done to enable computer, as brain of robot, to learn color categorization. Most of them rely on modeling of human color perception and mathematical complexities.

This work aims at developing the innate ability of the computer to learn the human-like color categorization. It focuses on the representation of color categorization and how it is built and developed without much mathematical complexity.

Keywords: color categorization, color learning, machine learning, color naming

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ON THE ANTI-KEKULÉ NUMBER OF LEAP-FROG FULLERENE

Jelena SEDLAR[1], Klavdija KUTNAR[2], Damir VUKIČEVIĆ[3]

[1]*Faculty of Civil Engineering & Architecture, University of Split,*
HR-21000 Split, Matice Hrvatske 15, Croatia
[2]*University of Primorska, SI-6000 Koper, Cankarjeva 6, Slovenia*
[3]*Department of Mathematics, University of Split , HR-21000 Split, Nikole Tesle 12, Croatia*

The Anti-Kekulé number of a connected graph G is the smallest number of edges that have to be removed from G in such way that G remains connected but it has no Kekulé structures. In this paper it is proved that the Anti-Kekulé number of all fullerenes is either 3 or 4 and that for each leap-frog fullerene the Anti-Kekulé number can be established by observing finite number of cases not depending on the size of the fullerene.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

***Course on*:**

BIOINFORMATICS OF INTRINSICALLY UNSTRUCTURED PROTEINS

István SIMON

Institute of Enzymology, Hungarian Academy of Sciences,
H-1518 P.O.Box 7, Budapest, H-1113 Karolina ut 29, Hungary

SOME CHEMICAL APPLICATIONS OF THE ZHANG-ZHANG POLYNOMIAL

Sonja STANKOVIĆ, Ivan GUTMAN

Faculty of Science, University of Kragujevac, P.O. Box 60, 34000 Kragujevac, Serbia

The Zhang-Zhang polynomial $\zeta(x)$ is a recently conceived combinatorial polynomial, associated with benzenoid molecules. Its inventors are the Chinese mathematicians Fuji Zhang and Heping Zhang, who originally named it "*Clar covering polynomial*". In 1996 and 1997, when the main mathematical papers by Zhang and Zhang were published in mathematical journals, $\zeta(x)$ did not attract the attention of chemists. Recently we try to make chemists familiar with $\zeta(x)$, and to establish its chemical applications.

The Zhang-Zhang polynomial provides a far-reaching algebraization of the Clar aromatic sextet theory. A *Clar cover* of a benzenoid hydrocarbon *B* is a Clar-type diagram in which all carbon atoms of *B* are covered by disjoint aromatic sextets and/or double bonds. If $z(B,k)$ is the number of Clar covers of *B* with exactly *k* aromatic sextets, then the respective Zhang-Zhang polynomial is defined as:

$$\varsigma(B,x) = \sum_{k \geq 0} z(B,k)\, x^k$$

If $\varsigma(B,x)$ is known, then one can easily deduce the number of Clar and Kekulè structures of *B*, as well as its Clar number. In particular, $\varsigma(B,0) = K(B)$, where $K(B)$ is the Kekulè structure count.

Our applications of the Zhang-Zhang polynomial are based on the following reasoning. If some property *P* of benzenoid molecules can be approximated by means of an expression $P(B) \approx f(K(B))$, which is equivalent to $P(B) \approx f(\varsigma(B,x))$ for x=0, then for some other values of *x,* the approximation $P(B) \approx f(\varsigma(B,x))$ may happen to be better.

This line of reasoning was pursued for *Dewar Resonance Energy* (DRE) and *Topological Resonance Energy* (TRE). The most remarkable findings of this investigation were that

DRE and TRE have a significantly different dependence on Kekulè- and Clar-structure-based features of the underlying benzenoid molecule, and

Clar-type structures have very little effect on the examined resonance energies.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

A PROGRESS ON ATIYAH-SUTCLIFFE GEOMETRIC CONJECTURES

Dragutin SVRTAN

Department of Mathematics, University of Zagreb, 10000 Zagreb, Croatia

In 2001 Sir M. F. Atiyah formulated a conjecture C1 and later with P. Sutcliffe two stronger conjectures C2 and C3. These conjectures, inspired by physics (spin-statistics theorem of quantum mechanics), are geometrically defined for any configuration of points in the Euclidean three space. The conjecture C1 is proved for n = 3, 4 and for general n only for some special configurations (M.F. Atiyah, M. Eastwood and P. Norbury, D. Đoković). Interestingly the conjecture C2 (and also stronger C3) is not yet proven even for arbitrary four points in a plane. So far we have verified the conjectures C2 and C3 for parallelograms, cyclic quadrilaterals and some infinite families of tetrahedra. We have also proposed a strengthening of the conjecture C3 for configurations of four points (Four Points Conjectures). For almost collinear configurations (with all but one point on a line) we propose several new conjectures (some for symmetric functions) which imply C2 and C3. By using computations with multi-Schur functions we can do verifications up to n = 9 of our conjectures. We can also verify stronger conjecture of Đoković which imply C2 for his nonplanar configurations with dihedral symmetry. This was done jointly with I. Urbiha.

Finally we mention that by minimizing a geometrically defined energy, figuring in these conjectures, one gets a connection to some complicated physical theories, such as Skyrmions and Fullerenes.

The speaker found recently two different methods, by which a general case of the Four Points Conjectures in three space and a planar hyperbolic version (of C2) for five points is verified.

1. Atiyah M, Sutcliffe P, The Geometry of Point Particles. *arXiv: hep-th/0105179* (32 pages).
2. Atiyah M, Sutcliffe P, Polyhedra in Physics, Chemistry and Geometry*, arXiv: math-ph/03030701* (22 pages).
3. Svrtan D, Urbiha I, Atiyah-Sutcliffe Conjectures for almost Collinear Configurations and Some New Conjectures for Symmetric Functions, *arXiv: math/0406386* (23 pages).
4. Svrtan D, Urbiha I,Verification and Strengthening of the Atiyah-Sutcliffe Conjectures for Several Types of Configurations, *arXiv: math/0609174* (49 pages).

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

CROSSLINKING EFFICIENCY OF COTTON CELLULOSE MONITORED BY DIFFERENT PHYSICAL-CHEMICAL METHODS AND GENETIC PROGRAMMING

Olivera ŠAUPERL[1], Karin STANA-KLEINSCHEK[1], Miran BREZOČNIK[2]

[1]*University of Maribor, Faculty of Mechanical Engineering, Laboratory for Characterization & Processing of Polymers, Smetanova 17, 2000 Maribor, Slovenia*
[2]*University of Maribor, Faculty of Mechanical Engineering, Laboratory for Intelligent Manufacturing Systems, Smetanova 17, 2000 Maribor, Slovenia*

In this study, a comparison of crosslinking effect on alkaline treated as much as alkaline untreated and with different mass fractions of 1,2,3,4, Butanetetracarboxylic acid (BTCA) crosslinked cotton fibres was made with different physical-chemical methods. Using FT-IR spectroscopy degree of crosslinking was determined on the basis of the intensity of the bands at fixed wavelength numbers in relation to the referential band. The correlation between the accessibility and the reactivity of hydroxyl groups of cotton cellulose fibers and the crosslinking efficiency was investigated using the water retention capacity method and tensiometry. A comparison of accessible carboxyl groups amount into mercerized as much as unmercerized and with different mass fractions of BTCA crosslinked cotton fibres was made applying methylene blue method. On the basis of the experimental data which were obtained with the separate physical-chemical methods, different prediction models for crosslinking efficiency has been developed. Modelling has been taken out with the *Genetic Programming* (GP) method. Genetic programming is, similarly as genetic algorithm, the evolutionary computation method which imitates biological evolution of living organisms (*Figure 1*). In GP the structure subject to adaptation is the population of hierarchically organized computer programs. Since GP is a general optimization approach, it has been successfully applied for solving a wide range of different problems. Genetic programming results show good accordance with experimental data. However, the proposed approach for crosslinking prediction with GP is in this level of research used as an idea to precisely describe a very complicated system in case of a higher number of measurements as well as higher number of input variables influencing crosslinking capacity.

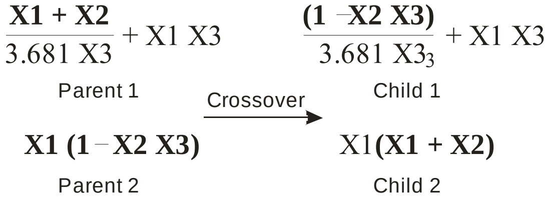


Figure 1. Crossover of two mathematical expressions

1. Šauperl O, Stana-Kleinschek K, Vončina B, Sfiligoj-Smole M, Majcen Le Marechal A (2003) Application of spectrophotometric methods in assessing the influence of alkaline treatment on the degree of crosslinking of cotton cellulose with BTCA, *Croat. Chem. Acta* **76** (4), 293-298.
2. Brezočnik M, Balič J, Brezočnik Z (2003) Emergence of intelligence in next-generation manufacturing systems*, Robot Comput Integrated Manuf.* **19**(1-2), 55-63.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

MODELLING OF EPITOPE-PARATOPE INTERACTION USING MOLECULAR RECOGNITION THEORY

Nikola ŠTAMBUK, Paško KONJEVODA, Dražen VIKIĆ-TOPIĆ, Biserka POKRIĆ

Ruđer Bošković Institute, HR-10002 Zagreb, Bijenička cesta 54, POB 180, Croatia

We investigated the modelling of epitope-paratope interactions using *Molecular Recognition Theory*. It is shown that the standard algorithm according to Kyte and Doolittle may be combined with complex methods of the secondary structure prediction to extract the information relevant for the epitope location and modelling. Described concept represents useful and simple set of procedures for deriving new biologically active peptides and antibodies and also performing modulation of peptide-receptor interaction.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

K OPERATOR: A NEW APPROACH TO DERIVE MOLECULAR DESCRIPTORS FROM GRAPH THEORETICAL MATRICES

Roberto TODESCHINI

Department of Environmental Sciences, University of Milano-Bicocca, 20126 Milano, Italy

The multivariate *K* correlation index was proposed in 1997 with the aim to evaluate the correlation content of a set of multivariate data. This index was demonstrated to be the exact measure of the whole multivariate correlation in a data set and several applications were proposed for variable reduction, regression model evaluation, mutlivariate information content, etc.

Now the same approach is proposed applying the *K* correlation operator to graph theoretical matrices and deriving new molecular descriptors. Some examples will be also given.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

THE EFFECTS OF SLOW AND FAST CLASSICAL MUSIC ON PHYSICAL AND MENTAL EXHAUSTION IN NON ATHLETE GIRL STUDENTS

Farnaz TORABI, Rahman SOORI, Ahmad FAROKHI

Physical Education Faculty, Tehran University of Iran, Tehran, Iran

Recent researches showed there are many factors that can affect motor performance and one of the most important them can be music. The aim of this research is to consider the effects of slow, fast classical music on physical, mental fatigue degree in girl students of general physical education Course in the 2^{nd} term of 84-85. In order to perform this study, 36 non athlete students aged 23±2 years were chosen randomly. A pretest was performed on subjects in a way that pedaling on ergometer cycle was executed in a 20 Watt power, then after each minute, 10 Watts was added to workload so that they became exhausted. According to the pretest data, subjects were devided in 3 groups (slow music, fast music and control) with 12 subjects in each one. Two experimental groups were doing the exercise as they listened to music by headphone. Exercise period included 5 weeks and 2 sessions in a week. Finally post test was completed. In this research, in addition to measure physical and mental fatigue by the time to reach exhaustion, laboratory apparatus such as Finger Tapping Test and Chart for Continual Naming of Colors Test (made by Yagami International Company) were used. Music groups showed less physical and mental fatigue than control group. In order to analyze the data, one way variance analyzes was used. The results suggested that the classical music with slow and fast rhythm delayed the time to reach exhaustion subjects significantly ($p = 0/028$). Also, slow and fast classical music has a significant additive effect on final workload of subjects ($p = 0/022$). So far, slow and fast classical music has a significant additive effect on H.R of exhaustion of subjects ($p = 0/013$). There was no significant difference between fast and slow music for reaching to exhaustion time, final workload and H.R of exhaustion ($p = 0/916$, $p = 0/755$, $p = 0/360$). It is obvious that music and simultaneous exercise resulted in increased performance and enhanced the time to reach exhaustion. These results support the perceptual narrowing theory such as parallel informative processing (Rejesky, 1985) and Sterbruk Cues utilization theory.

Keywords: classical music, physical, mental, fatigue, non athlete

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ON THE LEVELS OF MULTIPLE DEGENERACY: INTRINSIC MULTIPLICITY EXEMPLIFIED BY THE SIMPLEST SEMIREGULARLY AND IRREGULARLY DEGENERATE REARRANGEMENTS

Serge S. TRATCH, Marina S. MOLCHANOVA, Nikolai S. ZEFIROV

Chemistry Department of the Moscow State University, Moscow 117992, Russia

Topology graphs (and their labelings) were recently applied[1] to systematization of constitutionally degenerate interconversions of organic structures. The edges of the lower level topology graphs correspond only to bonds that change their multiplicity. At the medium and upper level, the unchanged bonds forming cycles and unchanged bonds forming substituents are also taken into account. In the present lecture, it is shown that *multiply degenerate* transformations (i.e., those representing interconversions of more than two identical structures) can be classified similarly. For this purpose, the corresponding *supertopology graphs* should be used. The multiple degeneracy of medium and upper levels is actually well-known. In all examples, the multiplicity is caused by unchanged bonds that form either cycles or substituents. For illustration purposes, several known multiply degenerate rearrangements are discussed in the lecture.

At the first sight, the lower level (*intrinsic*) multiple degeneracy cannot be represented by rearrangements because all known degenerate isomerization reactions are self-inverse and hence are always ordinarily degenerate. However, this level is shown to be realized by the theoretically predicted[2] highly specific degenerate interconversions. Contrary to traditional *regular* (*R*) degeneracy, the *semiregular* (*S*) and *irregular* (*I*) degeneracy cannot be associated with some automorphism(s) of the edge-labeled topology graph. The group theory formalism allowing to differentiate between *R*-, *S*-, and *I*-degenerate transformations is briefly explained in the lecture.

The smallest possible *S*- and *R*-degenerate rearrangements were found by means of our reaction-generating program ARGENT-1. The corresponding multiply degenerate transformations are characterized by original and edge-labeled topology/supertopology graphs and by corresponding reaction graphs, as well. The realizability problems for several unusual types of degeneracy and some open theoretical problems are finally mentioned.

1. Tratch SS, Molchanova MS, Zefirov NS (2005*) Croat. Chem. Acta* **79**, 339-353.
2. Tratch SS, Molchanova MS, ZefirovNS (2005*) Book of Abstracts MATH/CHEM/COMP 2005*, Dubrovnik, June 20-25, 2005; p. 72.

GRID-ENABLED PARALLEL FOCK MATRIX CONSTRUCTION

Hiroaki UMEDA[1,2], Yuichi INADOMI[3], Toshio WATANABE[1,2],
Takayoshi ISHIMOTO[1,2], Umpei NAGASHIMA[1,2]

[1] *CREST, Japan Science & Technology Agency, Kawaguchi, Saitama, 332-0012, Japan*
[2] *Research Institute for Computational Sciences, National Institute of Advanced Industrial Science & Technology, Tsukuba, Ibaraki, 305-8568, Japan*
[3] *Computing & Communications Center, Kyushu University, Sawara-ku, Fukuoka, 814-0001, Japan*

Parallel Fock matrix construction routine has been developed on the Grid using Ninf-G Grid programming middleware. Fock matrix construction is one of the most time consuming part in molecular orbital calculation, and it is hard to obtain molecular orbitals for large-scale molecular system unless using large-scale parallel computing. Ninf-G is the programming middleware managing GridRPC (*Grid Remote Procedure Call*) API with GlobusToolKit, and is suitable for large-scale scientific works on the Grid. For example, Ninf-G has functionality to call MPI program on the remote PC cluster system through GridRPC API. Using GridRPC/MPI hybrid communication model (*Figure 1*), we can easily handle hundreds of PCs on multiple PC cluster systems.

We have implemented Grid-enabled Fock matrix construction routine using Ninf-G. For efficient parallelization to handle heterogeneous computers on the Grid, we adopt dynamic load-balancing scheme between PC clusters, and within a PC cluster. The benchmark calculation with 512PU on three heterogeneous PC cluster systems (Xeon 3.06GHz 224PU, Xeon 3.06GHz 32PU, and Opteron246 2GHz 256PU in AIST Super Cluster system) shows efficient utilization of all 512PU on the Grid (*Figure 2*).

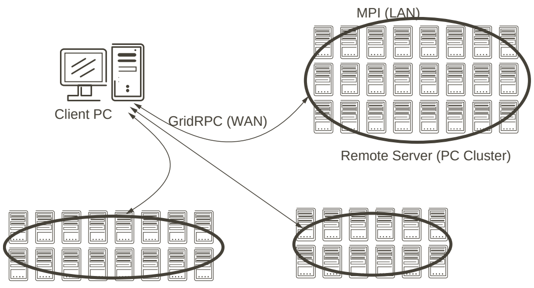


Figure 1. GridRPC/MPI hybrid communicaiton model

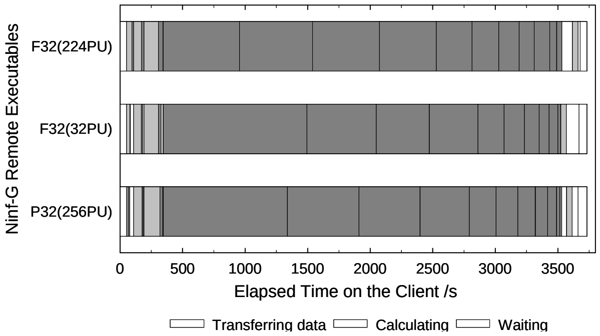


Figure 2. Ninf-G timing chart

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

GENERATING OF THE FIGURES OF SOME FULLERENES BY USING L-SYSTEM

Mehdi VAHIDIPOUR[1], Hosein SABAGHIAN-BIDOLI[1],
Gholam Reza VAKILI-NEZHAAD[2]

[1]*Department of Computer Engineering, University of Kashan, Kashan, Iran.*
[2]*Department of Chemical Engineering, University of Kashan, Kashan, Iran*

In 1968, Aristid Lindenmayer introduced a biologically motivated formalism for simulating the development of multi-cellular organisms, subsequently named L-systems. The applications include, on one hand, the modeling and visualization of plants at different levels of abstraction and for a variety of purposes, and on the other hand for geometric modeling of curves and surfaces.

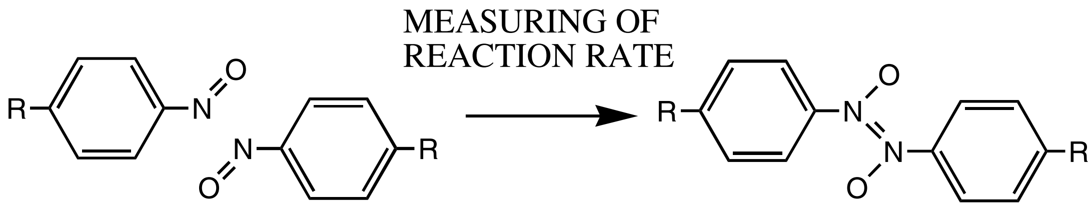
In this paper, we introduce L-system for generating figure of fullerenes C_{20} and C_{60}, without information about the carbon coordinates. We choose L-systems because they can express drawing steps in a compact way and are parallel in nature. They can be also used for visualizing of complex supramolecules.

CONCEPT FOR THE SOLID STATE REACTION MECHANISM

Hrvoj VANČIK

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102A,
HR-10000 Zagreb, Croatia

Thermal dimerization of different nitrozobenzene derivatives is applied as a molecular model for a systematic approach to the characterization of solid-state reaction mechanisms, which is based on kinetic relations between two processes, chemical reaction and phase transformation, respectively. We propose three basic reaction mechanisms in the formation of azodioxides from the corresponding nitrosobenzenes, a mechanism with the exponential first order type kinetics, in which the slow rate determining step is chemical reaction, two-step process where chemical reaction yields a metastable phase, which in the second step transforms to the final stable crystalline product phase, and the mechanism characterized with the sigmoid kinetics in which the rate determining phase transformation is much slower than the chemical reaction.



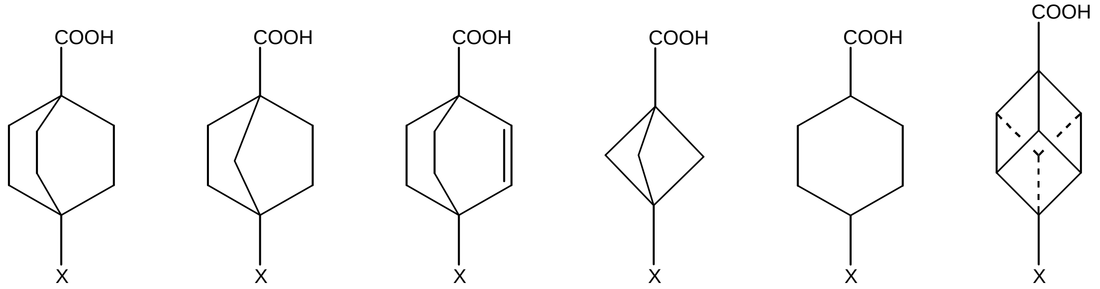
M **D**

MOLECULAR BASIS OF LFER: THEORETICAL STUDY OF POLAR SUBSTITUENT EFFECT IN ALIPHATIC SERIES

Sofie VAN DAMME[1], Robert PONEC[2]

[1]*Department of Inorganic & Physical Chemistry, Ghent University, Krijgslaan 281,*
9000 Gent, Belgium
[2] *Institute of Chemical Process Fundamentals, Czech Academy of Sciences, Prague 6,*
Suchdol 2, 165 -02, Czech Republic

This study contributes to the existing debate concerning the propagation of the inductive effect of substituents along molecular skeletons. The nature of the inductive effect is analysed by the systematic study of gas phase proton transfer equilibria in series of substituted aliphatic carboxylic acids with rigid molecular skeletons.



Our approach relies on the application of the recently proposed quantum chemical theory[1] based on the theory of proton affinity proposed by Longuet-Higgins.[2] Within this approach it is possible to partition the total proton affinity into two contributions which can be regarded as the theoretical counterparts of the classical concepts of field- and sigma inductive effect. The central aim of this study is to evaluate the factors responsible for the propagation of the inductive effect by comparing the transmission through the different skeletons.

The results of the analysis suggest that the dominant mechanism in the substituent induced variation of the acidity is the electrostatic field-effect which, in the gas phase, can reasonably be characterized by the Kirkwood-Westheimer theory.[3]

1. Ponec R, Girones X, Carbo-Dorca R (2002) *J. Chem. Inf. Comp. Sci.*, **42**, 564.
2. Longuet Higgins HC (1956) *Rec. Trav. Chim.* **75**, 825.
3. Kirkwood JG, Westheimer FW (1938) *J. Chem. Phys.* **6,** 506 and 513.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

NON EUCLIDEAN GEOMETRY-FACTS, FEATURES AND FUNS

Darko VELJAN

Department of Mathematics, University of Zagreb, HR-10000 Zagreb, Bijenička c. 30, Croatia

The common theme that links Plato, Archimedes, Kepler, Einstein, the quantum theorists and present-day string theorists is the belief that an understanding of the basic stuff of the universe will be found using mathematics. Sometimes, math runs ahead of physics. Today, however, the mathematicians are behind and trying to catch up. This situation is nothing new. Newton's investigations into mechanics (planet's motions, etc.) and optics led him to develop calculus.

More recently, Einstein's observations that gravity could be understood using a "strange" new kind of geometry developed earlier by Gauss, Lobachevsky, Bolyai, and in a unifying way by Riemann, led to the massive development of this geometry and its rapid incorporation into mainstream mathematics.

In this talk we shall discuss Lobachevsky geometry (also called hyperbolic) and Riemannian (elliptic) geometry. Riemannian geometry locally (in the small) coincides with the geometry of the sphere in ordinary three-dimensional space, and theorems of spherical geometry can be interpreted as ordinary space geometry theorems.

In Lobachevsky geometry, through any point not belonging to a line, one can draw many lines disjoint with the given line. For many centuries, people could not believe that this was possible. Euclid's fifth postulate (through any point not on a line there is only one parallel to that line) seemed to be a theorem following from the other axioms. This belief proved to be false. The basic theorems of hyperbolic geometry were proved by the above mentioned mathematicians, and then followed by Beltrami, Cayley, Klein who Poincare who constructed models of this geometry, and the reality of this non-Euclidean geometry became evident.

Beside showing some fundamental facts about these geometries, we shall also present some original results concerning some basic triangle inequalities. The first is the cosine-law type inequality in all three geometries. We further present the non-Euclidean version of the well known Euler's inequality ($R > 2r$), Finsler-Hadwiger's inequality and the "fundamental triangle inequality".

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

THE TRUE FAMILY OF C_{60}

Aniela E. VIZITIU[1], Simona CHIGER[1], Margareta S. FLORESCU[2], Mircea V. DIUDEA[1]

[1]*Babes-Bolyai University, Faculty of Chemistry & Chemical Engineering, 400028 Cluj, Romania*
[2]*Academy of Economic Sciences, Bucharest, Romania*

Map operations[1,2] are useful tools to transform any polyhedral tessellations. Using such operations, a family of fullerenes, having a perfect Clar PC structure (*i.e.*, a 2-factor) consisting of only pentagons, was modeled. The well-known C_{60} fullerene (*Figure 1*) is the smallest member of this family. All the members of this family show close properties:

(i) a covering by joint sumanenic flowers (see also *Figure 2*), and

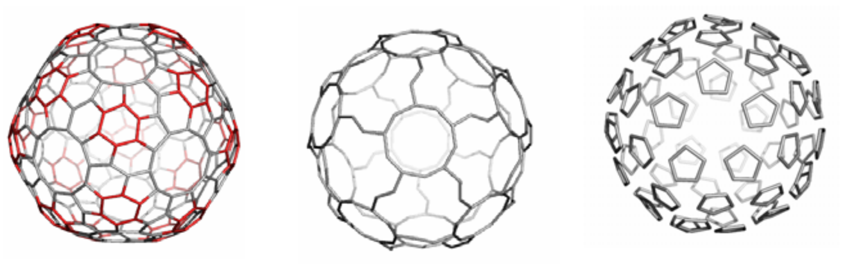
(ii) a very good stability.[3,4]

Related fullerenes showing disjoint sumanenic flowers are also given.[5]

v= 60; 4×[6:(5,6)$_3$]JFw & 4×JR$_6$
K :(3(0,3)^3) & (3)

4×[6:(5,6)$_3$]co-JFw & 4×JR$_6$
K :(3(0,3)^3) & (3)

Figure 1. Sumanenic patterns in a tetrahedral embedding, as in C_{60}



v= 300; 20×[6:(5,6)$_3$]JFw & 12×JR$_{10}$

Joint contours

Perfect Clar (2-factor)

Figure 2. Sumanenic patterns in a dodecahedral embedding, as in C_{300}

1. Pisanski T, Randić M (2000) Bridges between geometry and graph theory, in: *Geometry at Work: A Collection of Papers Showing Applications of Geometry* (Gorini CA, ed.), *Math. Assoc. Amer*. **53**, 174-194.
2. Diudea MV (2004) Covering forms in nanostructures, *Forma* (Tokyo) **19**, 131-163.
3. FowlerPW, Steer JI (1987) The leapfrog principle: a rule for electron counts of carbon clusters, *J. Chem. Soc. Chem. Commun*. **1987**, 1403-1405.
4. Diudea MV (2007) Retro-Leapfrog and structure elucidation, *J. Math. Chem*., in press.
5. Diudea MV, Nagy CL (2007) *Periodic Nanostructures*, Springer.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

ON THE VALENCE CONNECTIVITY IN TREES

Damir VUKIČEVIĆ[1], Ivan GUTMAN[2]

[1]*Department of Mathematics, University of Split, N. Tesle 12, HR-21000 Split, Croatia*
[2]*Faculty of Science, University of Kragujevac, P.O. Box 60, 34000 Kragujevac, Serbia*

Let $m_{ij}(G)$ be the number of edges of a graph *G*, connecting vertices of degrees i and j. Necessary and sufficient conditions are established for a sequence of numbers μ_{ij} such that there is a tree *T* for which $\mu_{ij} = m_{ij}(T)$ holds for all *i,j*.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

TREES WITH MAXIMAL ZAGREB INDEX AND PRESCRIBED NUMBERS OF VERTICES OF GIVEN DEGREE

Damir VUKIČEVIĆ[1], Sarah Michele RAJTMAJER[2]

[1]*Department of Mathematics, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia*
[2]*Department of Mathematics, University of Zagreb, Bijenička 30, HR-10002 Zagreb, Croatia*

A simple algorithm for calculating the maximal value of the Zagreb index for trees with prescribed number of vertices of given degree is presented. As the user inputs values n_1, n_2,....., n_Δ, , where n_i is the number of vertices of degree i, the algorithm outputs the maximal value of the Zagreb index. The complexity of the algorithm is proportional to Δ^3, where Δ is maximal degree, and is independent on the number of vertices. This means that for chemical trees with $\Delta \leq 4$, the algorithm works in constant time no matter how large the molecule is.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

RECURRENT APPROXIMATION OF PHYSICOCHEMICAL PROPERTIES OF HOMOLOGUES OF ORGANIC COMPOUNDS. ANALOGY WITH RECURSIVE NUMERICAL SEQUENCES

Igor G. ZENKEVICH

Research Institute of Chemistry, St. Petersburg State University,
St. Petersburg 198504, Universitetsky pr., 26, Russia

During 2005-2006 it was estimated that variations of most of physicochemical properties of organic compounds (A) within homologous series can be approximated by simplest first order recurrent relationship (correlation coefficients exceed 0.999):[1,2]

A(n+1) = *a* A(n) + *b* (*1*)

where n is the number of carbon atoms in the molecule.
It is noteworthy that eq. (1) describes not only the variations of different physicochemical constants of homologues within every series. Single recurrent equations can be used in approximation of various constants of all series or organic compounds with the same homologous differences. For example, parameters of recurrency (1) for normal boiling points are equal:

Homologous difference CH_2: $a = 0.930 \pm 0.002$, $b = 33.5 \pm 0.3$, $r = 0.9995$, $S_0 = 2.4$
Homologous difference CF_2: $a = 0.893 \pm 0.005$, $b = 32.1 \pm 0.3$, $r = 0.9997$, $S_0 = 1.9$

This general character of recurrences in organic chemistry requires explanations.

Lemma:
If recurrent numerical sequence in defined by linear equation of second (or higher) orders:
$A(n) = a\,A(n-1) + bA(n-2) + \ldots + w$
it can be approximated by linear recurrent equation of the first order:
$A(n) = a'\,A(n-1) + b'$

Comparison of Fibonacci and Lucas numbers:

Fibonacci numbers:
F(0) = 0, F(1) = 1, F(n) – F(n-1) + F(n-2), i.e. 0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, …
Parameters of recurrence (1): $a = 1.618 \pm 0.000$ (golden section), $b = -0.02 \pm 0.04 \sim 0$, $r = 1.0$, $S_0 = 0.16 \to 0$.

Lucas numbers:
L(0) = 2, L(1) = 1, L(n) = L(n-1) + L(n-2), i.e. 2, 1, 3, 4, 7, 11, 18, 29, 47, 76, 123, 199, 322, …
Parameters of recurrence (1): $a = 1.618 \pm 0.000$ (golden section), $b = 0.04 \pm 0.04 \sim 0$, $r = 1.0$, $S_0 = 0.18 \to 0$.

Therefore, the following analogy could be taken into account:

Numerical sequences in mathematics	Homologous series in chemistry
Initial conditions	Different physicochemical properties
General rule of sequence	Variations of properties within series with the same homologous difference

Similar processing of other numerical sequences (e.g., Padovan and Perrin numbers) confirms that values of coefficients of recurrent relation (1) indicate no dependence on their initial conditions. These coefficients are determined only by the general rule of sequences that is one of the explanations of the universal character of recurrent approximation of homologous properties.

1. Zenkevich IG (2005) *Lect. Ser. Comput. Comput. Sci.* **4**, 1574-1577.
2. Zenkevich IG (2006) *J. Org. Chem. Rus.* **42**, 9-20.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

HAMILTONICITY AND THE CATACONDENSED BENZENOID GRAPHS

Petra ŽIGERT

Faculty of Chemistry & Chemical Engineering, University of Maribor, SI-2000 Maribor, Slovenia

The vertex set of the resonance graph R(B) of a benzenoid graph B consists of 1-factors of B, i.e. the resonance structures of B, two 1-factors being adjacent whenever their symmetric difference forms the edge set of a single hexagon of B. Graph G is hamiltonian if it admits a Hamilton cycle,i.e. a cycle that contains all of graph vertices. For some time it is known that for a catacondensed benzenoid graph the corresponding R(B) contains a Hamilton path.

In order for R(B) to admits a Hamilton cycle it must be of even order with the minimal degree of a graph greater than 1. We show that for a class of catacondensed benzenoid graphs this necessary condition is also the sufficient condition for the existence of a Hamilton cycle. The construction of such a cycle is outlined.

Abstract: MATH/CHEM/COMP 2007, Dubrovnik, June 11-16, 2007

EXACT TREATMENT OF OPEN QUANTUM SYSTEMS

Tomislav ŽIVKOVIĆ

Ruđer Bošković Institute, Bijenička 54, HR-10002Zagreb, P.O.B. 180, Croatia

One of the most important mathematical problems in quantum theory is an exact treatment of open quantum systems, i.e. such quantum systems that interact with surrounding (whatever this surrounding may be). Usually, such open system can be very well approximated as a finite quantum system, i.e. as quantum system with finite number of eigenvalues and eigenstates. Typical examples of such open quantum systems are:

(a) isolated molecule that interacts with the electromagnetic field,
(b) molecule adsorbed on some surface that interacts with this surface,
(c) interaction of a molecule with a solute in which it is dissolved, etc.

There are generally two main methods how such problems are treated. If the interaction of this system with its surrounding is relatively weak, one can treat this interaction using the formalism of the perturbation expansion. The interaction of a molecule with the electromagnetic field is usually treated in this way. Quantum description of this interaction is the main subject of spectroscopy. However, if highly reliable results are needed, perturbation expansion may converge unacceptably slow and in this case such an approach is not satisfactory. In addition, if the interaction of quantum system with its surrounding is strong, perturbation expansion usually diverges. Typical example is the interaction of a molecule in a solution with the solute or the interaction of a molecule adsorbed on some surface with this surface. In this case one has to use some semi-classical model. However, such an approach is only approximate and it can never completely replace exact quantum treatment. A new mathematical formalism for the exact treatment of the interaction of a finite quantum system with its surrounding (however complicated) will be presented. In particular, it will be shown that a finite quantum system interacts with only a small fraction of its surrounding. A huge fraction of this surrounding is completely (and exactly) unaffected by this interaction. Since this surrounding is as a rule an infinite quantum system (e.g. electromagnetic field is an infinite quantum system with an infinite number of degrees of freedom), the problem of the interaction of a finite quantum system with its surrounding can be reduced (exactly) to a mathematically much simpler problem.