IISER Mohali Research Publications Bulletin No. 1

Annotated Bibliography of
IISER Mohali
Research Publications
2007 – 2012

Compiled and Edited by

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Published by : Director, Indian Institute of Science Education and Research (IISER) Mohali
Knowledge City, Sector-81, SAS Nager, Manauli (P.O), Mohali - 140306, Punjab , India

Printed by : Skill Spot, Shop # 74, Sector- 16 D., Chandigarh -160015, India

Foreword

I am delighted to see this compilation of research publications from IISER Mohali for the first five years of its existence. The Indian Institutes of Science Education and Research (IISERs) were established by the Government of India to give an impetus to research in the country and to inculcate a research culture at the undergraduate level. The establishment of IISERs is one of the conscious steps taken by the Government to keep India at the forefront of science.

Science is driven by curiosity, curiosity about us and our environment. Questions about everything in Nature are answered by carefully designed experiments and careful observations. The results are analysed and interpreted to understand Nature and its functioning. Laws of Nature are arrived at and the understanding is used to improve the quality of life around us.

Although the society evaluates the scientific output in terms of the benefits to the society, the scientific community measures it through publications that are evaluated by the peers. As was pointed out by Michael Faraday, any research is not complete until the results are analysed and reported in the form of publications.

One of the tangible outcomes of the funds invested in IISER Mohali is the research publications. The Institute started functioning with one faculty member (the founder Director) in the year 2007 and there was only one research publication that year. In the subsequent five years, the faculty strength went up to approximately 60 and the number of research publications increased several fold. The publications include books on topics of contemporary interest and from interdisciplinary areas. Particularly satisfying is the fact that most of these publications have risen out of the research carried out by the PhD students and a significant number by the undergraduates. Research has become a way of life at IISER Mohali and this is reflected in its research publications.

I congratulate Dr. P. Visakhi, Deputy Librarian for putting such a document together.

N. Sathy

(N. Sathyamurthy)
Director, IISER Mohali

Mohali
May , 2013

Preface

The annotated bibliography is a traditional form of " Abstract Database " which gives alphabetical listing of bibliographic data of Publications. In addition to bibliographic data, an annotated bibliography provides a concise summary of each Publication and some assessment of its value or relevance. This bibliography covers the research articles/ Books / book Chapters etc published by IISER Mohali research Community from 2007 to 2012. The "Master list" of 218 references has been brought out after filtering the bibliographical references drawn from the primary and secondary sources.

Each reference from the " Master list" was visited to its original source and verified with author's affiliation, title, pattern of contribution, year, Publisher, source, pagination etc. The Articles published with IISER Mohali"s affiliation were only considered to include in this bibliography. Even if IISER Mohali was given as " Present address' was also not considered for this publication. The refernces were included with minor changes where ever it is essential. Abstract has also been drawn from original source, however it has been observed that there was a discrepency in the format especially in Chemical formulas, structures like superscript and subscript and also Mathematical symbols. So it was taken utmost care to keep the originalty intact by typing the chemical formulas, symbols etc. The Keywords are taken from primary as well as secondary sources where ever it is appropriate to give more source of visibilty. URL (hyperlinks) are taken from original sources as well as secondary source such as Open access Institutional , Publishers' as well as Author 's Repositories.

The bibliographical information of "Master list' is arranged in "The Modern Language Association (MLA) Citation" Style and all references are categorized by year. Again within each year , the titles of references are organized " Alphabetically". The alphabetical list of Books Published by IISER Mohali research community is enlisted at the end of Master list along with Book description.

The indixes of IISER Mohali Author(s), Source as well as Publishers have been provided as an Annexures.

While bring out this Publication, the Compiler has taken all precautions to maintain the originality as well as error free. Despite all efforts , if any inadvertent mistake of any sort occurs, may kindly consider it as human error or technical error but not intentional.

Hope this Publication will be useful to the researchers as "Handy" and "Ready Reckoner".

I take this opportunity to acknowledge my sincere thanks and gratitude to ***Prof. N. Sathyamurthy,*** *Director, IISER Mohali for his suggestions and constant support during preparation of this Publication.*

With Best Wishes !!!

(P. Visakhi)
Compiler & Editor
Deputy Librarian, IISER Mohali

Mohali
May, 2013

Annotated Bibliography of IISER Mohali Research Publications

2007-2012

Contents

IISER Mohali Research Publications : 2007-2012

MASTER LIST

Titles : A - Z

2007

1. R. Parthasarathi., V.Subramanian., **N. Sathyamurthy** **(2007)** *Hydrogen bonding in protonated water clusters: An atoms-in-molecules perspective*. **Journal of Physical Chemistry A, 111 (51), pp. 13287-13290.**

ABSTRACT: This article highlights the results of a detailed study of hydrogen bonding in the first and the second solvation shells of Eigen (H_3O^+) and Zundel ($H_5O_2^+$)cations solvated by water in a stepwise manner. It is evident from the results that an electron density analysis clearly distinguishes the first and the second solvation shell and helps in quantifying the strength of hydrogen bonding in these clusters. © 2007 American Chemical Society.

KEYWORDS: Carrier concentration; Molecular structure; Protonation; Solvation; Water, Protonated water clusters; Solvation shells, Hydrogen bonds

http://pubs.acs.org/doi/abs/10.1021/jp0775909

DOI:10.1021/jp0775909

Titles
A - Z : 2008

2008

2. Mishra, B.K., Bajpai, V.K., Ramanathan, V., Gadre, S.R., **N.Sathyamurthy (2008)** *Cation-π interaction: To stack or to spread.* **Molecular Physics, 106 (12-13), pp. 1557-1566.**

ABSTRACT: The interaction between different cations and certain aromatic dimers (benzene, naphthalene, anthracene) and heteroaromatic dimers (pyridine, pyrazine, *sym*-triazine and *sym*-tetrazine) has been investigated employing the MP2 level of theory with the 6-31G** and 6-311++G** basis sets. The trend in the stabilization energy for aromatic dimers is found to be: $(\text{anthracene})_2$-cation>$(\text{naphthalene})_2$-cation>$(\text{benzene})_2$-cation. In all three cases, the cation remains sandwiched between the rings. In the case of the heteroaromatic systems, on the other hand, the cation prefers to interact with the nitrogen atom of the ring. These results can be rationalized by molecular electrostatic potential maps for the systems under consideration. In addition, these results are in conformity with the available cation aromatic database.

KEYWORDS: Aromatic compounds; Benzene; Flow interactions; Naphthalene; Oligomers; Polycyclic aromatic hydrocarbons; Positive ions, Pyrazine; Spreading interaction; Stacking interaction; Tetrazine, Dimers

http://www.tandfonline.com/doi/abs/10.1080/00268970802175290

DOI:10.1080/00268970802175290

3. Sangeeta Chakrabarti., S. **Anantha Ramakrishna**, Harshawardhan Wanare **(2008)** *Coherently controlling metamaterials*. **Optics Express, 16 (24), pp. 19504-19511.**

ABSTRACT: Two independent significant developments have challenged our understanding of light-matter interaction, one, involves the artificially structured materials known as metamaterials, and the other, relates to the coherent control of quantum systems via the quantum interference route. We theoretically demonstrate that one can engineer the electromagnetic response of

composite metamaterials using coherent quantum interference effects. In particular, we predict that these composite materials can show a variety of effects ranging from dramatic reduction of losses to switchable ultraslow-to-superluminal pulse propagation. We propose parametric control of the metamaterials by active tuning of the capacitance of the structures, which is most efficiently engineered by embedding the metamaterial structures within a coherent atomic/molecular medium. This leads to dramatic frequency dependent features, such as significantly reduced dissipation accompanied by enhanced filling fraction. For a Split-ring resonator medium with magnetic properties, the associated splitting of the negative permeability band can be exploited for narrow band switching applications at near infrared frequencies involving just a single layer of such composite metamaterials. © 2008 Optical Society of America.

KEYWORDS: Control systems; Magnetic properties; Materials science; Optical resonators; Quantum electronics; Quantum interference devices; Quantum interference phenomena; Quantum optics, Artificially structured materials; Coherent controls; Composite metamaterials; Electromagnetic responses; Filling fractions; Frequency dependents; Metamaterial structures; Metamaterials; Narrow bands; Near infrared; Negative permeabilities; Parametric controls; Quantum interferences; Quantum systems; Ring resonators; Single layers; Superluminal pulse propagations; Switchable; Switching applications, Electronic equipment

http://www.opticsinfobase.org/oe/fulltext.cfm?uri=oe-16-24-19504&id=174462

http://dx.doi.org/10.1364/OE.16.019504

4. Manash K. Paul., Rajinder K., Anup K. Mukhopadhyay (**2008)** *Characterization of rat liver mitochondrial permeabilty transition pore.* **African Journal Pharmacy & Pharmacology , 2 (2) pp.14-21**

ABSTRACT : The mitochondrial permeability transition (MPT) is considered to contribute substantially to the regulation of normal mitochondrial metabolism and plays as an important mediator of cell death. MPT is regulated in a tissue specific manner. The importance of this work is highlighted by the fact that knowledge regarding liver MPT may serve as important determinants of the physiological state of the liver. Our results suggest that liver mitochondria exhibit a cyclosporin A sensitive, exogenous calcium mediated full scale MPT opening, indicative of classical MPT. Transmission electron microscopy suggests a homogeneous mitochondrial population. Complex II substrate (succinate) in comparison to complex I substrate (NADH) induces increased MPT opening. Reactive Oxygen Species induces liver mitochondrial MPT opening and is abrogated by ascorbic acid and #-tocopherol. Liver MPT is sensitive to redox modulation. Reducing and oxidizing agents decrease and increase MPT opening respectively. MPT of liver mitochondria show typical pH dependence, acidic and alkaline pH induces MPT closure while, maximal MPT opening and calcium sensitivity was achieved at a pH range of ~7.2-7.4. ATP inhibited, while ADP activated MPT opening. Thus, our study demonstrates that all the major MPT functions in normal liver mitochondria could be determined by simple mitochondrial swelling assay under well-defined conditions, thereby suggesting its application in therapeutic diagnostics.

KEYWORDS : Mitochondria, mitochondrial permeability transition, swelling assay, oxidants, reductants, calcium, cyclosporin A, pH.

http://www.academicjournals.org/ajpp/PDF/pdf2008/Apr/Manash%20et%20al.pdf

5. Shubbir Ahmed., Divya Kapoor., Balvinder Singh., **Purnananda Guptasarma (2008)** *Conformational behavior of polypeptides derived through simultaneous global conservative site-directed mutagenesis of chymotrypsin inhibitor 2*. **Biochimica et Biophysica Acta - Proteins and Proteomics, 1784 (5), pp. 796-805.**

ABSTRACT: The natural occurrence of conservative residue substitutions in proteins suggests that side-chain packing schemes in protein interiors can accommodate mutational replacements of residues by others of similar nature. To explore the extent to which such substitutions are tolerated, especially when introduced simultaneously and globally over the entire length of a polypeptide chain, we examined the conformational behavior of a model 65 residues-long protein, wild-type chymotrypsin inhibitor 2 (WTCI2), and two globally-mutated (GM) variants named GMCI2-1 and GMCI2-2, each incorporating 55

conservative residue substitutions. GMCI2-1, was soluble over a wide range of pH, and folded into a compact, spherical, monomer marked by (i) complete absence of surface hydrophobicity, (ii) a WTCI2-like betaII-type CD spectrum, (iii) high WTCI2-like thermal stability, and (d) 1D and 2D NMR spectra characteristic of folded protein structure. GMCI2-2 was insoluble over a wide range of pH, and could be solubilized only at pH 4.0, showing non-WTCI2-like far-UV CD spectra characterized by high helical content. These results tentatively indicate that polypeptides incorporating residues of identical nature at equivalent chain locations can show the potential to fold with similar characteristics. However, further detailed investigations would be required to determine whether indeed the structural fold of GMCI2-1 resembles that of WTCI2, and to evaluate the extent to which it does so. © 2008 Elsevier B.V. All rights reserved.

KEYWORDS: chymotrypsin inhibitor; chymotrypsin inhibitor 2; polypeptide; unclassified drug, article; genetic variability; globally mutated variant; hydrophobicity; mutagenesis; nuclear magnetic resonance spectroscopy; pH; priority journal; protein conformation; protein structure; solubility; thermostability; ultraviolet radiation; wild type, Amino Acid Sequence; Chromatography, Gel; Circular Dichroism; Heat; Hydrophobicity; Magnetic Resonance Spectroscopy; Models, Molecular; Molecular Sequence Data; Mutagenesis, Site-Directed; Mutant Proteins; Peptides; Plant Proteins; Protein Conformation; Protein Folding; Recombinant Proteins; Solubility; Subtilisin; Thermodynamics; Tryptophan

http://www.sciencedirect.com/science/article/pii/S1570963908000435

http://dx.doi.org/10.1016/j.bbapap.2008.01.023

6. Shubbir Ahmed., **Purnananda Guptasarma (2008)** *Design of a soluble mini-protein through tandem duplication of the minimally engineered beta hairpin 'tongue' motif of alpha-hemolysin.* **Biochimie, 90 (6), pp. 957-967.**

ABSTRACT: In an attempt to fashion a globular protein out of two conjoined beta hairpin structural motif(s), we created a gene encoding, in tandem, two copies of the 40 residues-long transmembrane beta hairpin tongue (BHT) motif of the pore-forming toxin, alpha-hemolysin, of Staphylococcus aureus. Seven selected hydrophobic residues on each copy of the BHT motif's lipid-facing surface were mutated to hydrophilic residues, to prevent or reduce any non-specific aggregation based on hydrophobic interactions. Tandem BHT turned out to be expressed as a soluble polypeptide which could be raised to concentrations of ~2 mg/ml. It displayed several characteristics of a folded mini-protein, although not the characteristics of a typical well-folded globular protein. These characteristics include (i) far-UV CD and FTIR spectra indicative of the presence of sheet structure mixed with polyproline type II secondary structure, (ii) a near-UV CD spectrum, indicating some formation of tertiary structure, (iii) evidence of unfolding and dissociation transitions in the presence of denaturants, accompanied by increase in random coil content, and (iv) the ability to transform from sheet to helical structure through a biphasic structural transition in the presence of the cosolvent, trifluorethanol. Importantly, however, tandem BHT displayed no cooperativity during unfolding; taken together with the poor structural content revealed in the far-UV CD spectrum and some non-canonical gel filtration behavior seen in the presence of denaturants, this suggests a partially unsuccessful instance of protein design. © 2008 Elsevier Masson SAS. All rights reserved.

KEYWORDS: alpha hemolysin, amino acid sequence; article; concentration (parameters); gel filtration; protein folding; protein motif; protein structure; Staphylococcus aureus, Amino Acid Motifs; Amino Acid Sequence; Bacterial Toxins; Circular Dichroism; Dimerization; Heat; Hemolysin Proteins; Molecular Sequence Data; Protein Denaturation; Protein Engineering; Protein Folding; Protein Structure, Secondary; Solubility; Solvents; Spectroscopy, Fourier Transform Infrared; Subtilisins, Staphylococcus aureus

http://www.sciencedirect.com/science/article/pii/S0300908408000680

http://dx.doi.org/10.1016/j.biochi.2008.02.024

7. **Manash K Paul.,** Rajinder Kumar., Anup K. Mukhopadhyay **(2008)** *Dithiothreitol abrogates the effect of arsenic trioxide on normal rat liver mitochondria and human hepatocellular carcinoma cells*. **Toxicology and Applied Pharmacology, 226 (2), pp. 140-152.**

ABSTRACT: Arsenic trioxide (ATO) is a known environmental toxicant and a potent chemotherapeutic agent. Significant correlation has been reported between consumption of arsenic-contaminated water and occurrence of liver cancer; moreover, ATO-treated leukemia patients also suffers from liver toxicity. Hence, modulation of ATO action may help to prevent populations suffering from arsenic toxicity as well as help reduce the drug-related side effects. Dithiothreitol (DTT) is a well-known dithiol agent reported to modulate the action of ATO. Controversial reports exist regarding the effect of DTT on ATO-induced apoptosis in leukemia cells. To the best of our knowledge, no report illustrates the modulatory effect of DTT on ATO-induced liver toxicity, the prime target for arsenic. Mitochondria serve as the doorway to apoptosis and have been implicated in ATO-induced cell death. Hence, we attempted to study the modulatory effect of DTT on ATO-induced dysfunction of mammalian liver mitochondria and human hepatocellular carcinoma cell line (Hep3B). We, for the first time, report that ATO produces complex I-mediated electron transfer inhibition, reactive oxygen species (ROS) generation, respiration inhibition, and ATO-induced ROS-mediated mitochondrial permeability transition (MPT) opening. DTT at low concentration (100µM and less) prevents the effect of ATO-induced complex I-malfunctions. DTT protects mitochondria from ATO-mediated opening of MPT and membrane potential depolarization. DTT also prevented ATO-induced Hep3B cell death. Thus, at low concentrations DTT abrogates the effect of ATO on rat liver mitochondria and Hep3B cell line. Therefore, the present result suggests, that use of low concentration of dithiols as food supplement may prevent arsenic toxicity in affected population. © 2007 Elsevier Inc. All rights reserved.

KEYWORDS: arsenic trioxide; dithiothreitol; reactive oxygen metabolite, apoptosis; article; carcinoma cell; cell death; cell line; controlled study; depolarization; human; human cell; leukemia cell; liver cell carcinoma; liver mitochondrion; liver toxicity; membrane permeability; mitochondrion; respiration depression, Animals; Antineoplastic Agents; Apoptosis; Arsenicals; Carcinoma, Hepatocellular; Cell Line, Tumor; Dithiothreitol; Dose-Response Relationship, Drug; Electron Transport Chain Complex Proteins; Environmental Pollutants; Humans; Liver Neoplasms; Male; Membrane Potential, Mitochondrial; Mitochondria, Liver; Oxides; Oxygen Consumption; Rats; Rats, Sprague-Dawley; Reactive Oxygen Species, Mammalia; Rattus.

http://www.sciencedirect.com/science/article/pii/S0041008X07004164

http://dx.doi.org/10.1016/j.taap.2007.09.020

8. Sanjeev Kumar Chandrayan., Neeraj Dhaunta., **Purnananda Guptasarma (2008)** *Expression, purification, refolding and characterization of a putative lysophospholipase from Pyrococcus furiosus: Retention of structure and lipase/esterase activity in the presence of water-miscible organic solvents at high temperatures*. **Protein Expression and Purification, 59 (2), pp. 327-333.**

ABSTRACT: A putative lysophospholipase (PF0480) encoded by the Pyrococcus furiosus genome has previously been cloned and expressed in Escherichia coli. Studies involving crude extracts established the enzyme to be an esterase; however, owing presumably to its tendency to precipitate into inclusion bodies, purification and characterization have thus far not been reported. Here, we report the overexpression and successful recovery and refolding of the enzyme from inclusion bodies. Dynamic light scattering suggests that the enzyme is a dimer, or trimer, in aqueous solution. Circular dichroism and fluorescence spectroscopy show, respectively, that it has mixed beta/alpha structure and well-buried tryptophan residues. Conformational changes are negligible over the temperature range of 30-80 °C, and over the concentration range of 0-50% (v/v) of water mixtures with organic solvents such as methanol, ethanol and acetonitrile. The enzyme is confirmed to be an esterase (hydrolyzing *p*-NP-acetate and *p*-NP-butyrate) and also shown to be a lipase (hydrolyzing *p*-NP-palmitate), with lipolytic activity being overall about 18- to 20-fold lower than esterase activity. Against *p*-NP-palmitate the enzyme displays optimally activity at pH 7.0 and 70 °C. Remarkably, over 50% activity is retained at 70 °C in the presence of 25% acetonitrile. The high organic solvent stability and thermal stability suggest that this enzyme may have useful biodiesel-related applications, or applications in the pharmaceutical industry, once yields are optimized. © 2008 Elsevier Inc. All rights reserved.

KEYWORDS: bacterial protein; lysophospholipase; solvent; water, amino acid sequence; article; biosynthesis; chemistry; dimerization; enzyme stability; enzymology; Escherichia coli; genetics; heat; isolation and purification; molecular genetics; molecular weight; pH; protein folding; protein secondary structure; protein tertiary structure; Pyrococcus furiosus, Amino Acid Sequence; Bacterial Proteins; Dimerization; Enzyme Stability; Escherichia coli; Heat; Hydrogen-Ion Concentration; Lysophospholipase; Molecular Sequence Data; Molecular Weight; Protein Folding; Protein Structure, Secondary; Protein Structure, Tertiary; Pyrococcus furiosus; Solvents; Water, Escherichia coli; Pyrococcus furiosus

http://www.sciencedirect.com/science/article/pii/S1046592808000636

http://dx.doi.org/10.1016/j.pep.2008.02.019

9. Bharti Bisht., Chinmoy S Dey **(2008)** *Focal Adhesion Kinase contributes to insulin-induced actin reorganization into a mesh harboring glucose transporter-4 in insulin resistant skeletal muscle cells*. **BMC Cell Biology, 9, art. no. 48** .

ABSTRACT: Background: Focal Adhesion Kinase (FAK) is recently reported to regulate insulin resistance by regulating glucose uptake in C2C12 skeletal muscle cells. However, the underlying mechanism for FAK-mediated glucose transporter-4 translocation (Glut-4), responsible for glucose uptake, remains unknown. Recently actin remodeling was reported to be essential for Glut-4 translocation. Therefore, we investigated whether FAK contributes to insulin-induced actin remodeling and harbor Glut-4 for glucose transport and whether downregulation of FAK affects the remodeling and causes insulin resistance. Results: To address the issue we employed two approaches: gain of function by overexpressing FAK and loss of function by siRNA-mediated silencing of FAK. We observed that overexpression of FAK induces actin remodeling in skeletal muscle cells in presence of insulin. Concomitant to this Glut-4 molecules were also observed to be present in the vicinity of remodeled actin, as indicated by the colocalization studies. FAK-mediated actin remodeling resulted into subsequent glucose uptake via PI3K-dependent pathway. On the other hand FAK silencing reduced actin remodeling affecting Glut-4 translocation resulting into insulin resistance. Conclusion: The data confirms that FAK regulates glucose uptake through actin reorganization in skeletal muscle. FAK overexpression supports actin remodeling and subsequent glucose uptake in a PI3K dependent manner. Inhibition of FAK prevents insulin-stimulated remodeling of actin filaments resulting into decreased Glut-4 translocation and glucose uptake generating insulin resistance. To our knowledge this is the first study relating FAK, actin remodeling, Glut-4 translocation and glucose uptake and their interrelationship in generating insulin resistance. © 2008 Bisht and Dey; licensee BioMed Central Ltd.

KEYWORDS: actin; focal adhesion kinase; glucose; glucose transporter 4; insulin; phosphatidylinositol 3 kinase; small interfering RNA, animal cell; animal cell culture; article; cellular distribution; confocal laser microscopy; controlled study; cytolysis; down regulation; enzyme localization; fluorescence microscopy; gene overexpression; gene silencing; gene translocation; genetic transfection; glucose transport; insulin resistance; muscle cell; nonhuman; plasmid; skeletal muscle; Western blotting; animal; cell culture; confocal

microscopy; enzymology; genetics; metabolism; microfilament; mouse; physiology; ultrastructure, 1-Phosphatidylinositol 3-Kinase; Actins; Animals; Cells, Cultured; Focal Adhesion Protein-Tyrosine Kinases; Gene Silencing; Glucose; Glucose Transporter Type 4; Insulin; Insulin Resistance; Mice; Microfilaments; Microscopy, Confocal; Microscopy, Fluorescence; Muscle, Skeletal; RNA, Small Interfering; Transfection.

http://www.biomedcentral.com/1471-2121/9/48/#

DOI:10.1186/1471-2121-9-48

10. Shubbir Ahmed, Anshuman Shukla., **Purnananda Guptasarma (2008)** *Folding behavior of a backbone- reversed protein: Reversible polyproline type II to β-sheet thermal transitions in retro-GroES multimers with GroES-like features*. **Biochimica et Biophysica Acta - Proteins and Proteomics, 1784 (6), pp. 916-923**.

ABSTRACT: The structural consequences of the reversal of polypeptide backbone direction (retro modification) remain insufficiently explored. Here, we describe the behavior of an engineered, backbone-reversed form of the 97 residues-long GroES co-chaperonin of Escherichia coli. FTIR and far-UV CD spectroscopy suggest that retro-GroES adopts a mixed polyproline type II (PPII)-beta-strand structure with a β II type CD spectrum similar to that of GroES. Gel-filtration chromatography reveals that the protein adopts trimeric and/or pentameric quaternary structures, with solubility retained up to concentrations of 5.0-5.5 mg/ml in aqueous solutions. Mutations inserting a single tryptophan residue as a spectroscopic probe at three different sites cause no perturbation in the protein's CD spectral characteristics, or in its quaternary structural status. The protein is cooperatively dissociated, and non-cooperatively unfolded, by both guanidine hydrochloride and urea. Intriguingly, unlike with GroES, retro-GroES is not unfolded by heat. Instead, there is a reversible structural transition involving conversion of PPII structure to β sheet structure, upon heating, with no attendant aggregation even at 90°C. Retro-GroES does not bind GroEL. In summary, some structure-forming characteristics of GroES appear to be conserved through the backbone reversal process, although the differential conformational behavior upon heating also indicates differences. © 2008 Elsevier B.V. All rights reserved.

KEYWORDS: chaperonin; guanidine; polypeptide; proline; urea, aqueous solution; article; beta sheet; circular dichroism; Escherichia coli; gel filtration chromatography; heating; infrared spectroscopy; nonhuman; priority journal; protein aggregation; protein conformation; protein folding; protein quaternary structure; protein structure; solubility; ultraviolet spectroscopy, Chromatography, Gel; Circular Dichroism; Dimerization; Electrophoresis, Polyacrylamide Gel; Escherichia coli Proteins; GroEL Protein; GroES Protein; Peptides; Protein Conformation; Protein Folding; Spectrometry, Fluorescence; Spectrometry, Mass, Matrix-Assisted Laser Desorption-Ionization; Spectroscopy, Fourier Transform Infrared; Temperature; Thermodynamics, Escherichia coli

http://www.sciencedirect.com/science/article/pii/S1570963908000721

http://dx.doi.org/10.1016/j.bbapap.2008.02.009

11. C.N. Ramachandran., Debmalya Roy., **N. Sathyamurthy (2008)** *Host-guest interaction in endohedral fullerenes*. **Chemical Physics Letters, 461 (1-3), pp. 87-92**.

ABSTRACT: Ab initio calculations using Hartree-Fock (HF) and second order Møller-Plesset perturbation (MP2) theoretic methods using the 6-31G basis set have been used to study the interaction between H_+, H_-, He, Li_+ and H^2 with C60 fullerene. The barrier for penetration of the guest species through the center of the hexagon of the cage is reported. There is a substantial change in the HOMO-LUMO energy gap for the endohedral complex of $C^6$0 fullerene when the proton or hydride ion is encapsulated. The calculated HOMO-LUMO energy gap for the endohedral complex is correlated with the orbital energy of the guest species. The interaction of the guest species with the host is examined by a critical point analysis using Bader's theory of atoms in molecules. The effect of the guest species on the electrostatic potential inside and outside of the $C^6$0 cage is also discussed. © 2008 Elsevier B.V. All rights reserved.

KEYWORDS: Drug interactions; Flow interactions; Fullerenes, ab initio calculations; Basis sets; Endohedral fullerenes; Hartree Fock (HF); Host-guest interactions; Second orders, Calculations

http://www.sciencedirect.com/science/article/pii/S0009261408008907

http://dx.doi.org/10.1016/j.cplett.2008.06.073

12. Tapan K. Mukherjee., Srirupa Mukhopadhyay., John R. Hoidal **(2008)** I*mplication of receptor for advanced glycation end product (RAGE) in pulmonary health and pathophysiology* .**Respiratory Physiology and Neurobiology, 162 (3), pp. 210-215.**

ABSTRACT: Receptor for advanced glycation end products (RAGE) is a membrane bound receptor and member of the immunoglobulin super family and is normally present in a highly abundant basal level expression in lung. This high expression of RAGE in lung alveolar epithelial type I (ATI) cells is presumably involved in the proliferation and differentiation of pulmonary epithelial cells. However, typically higher than basal level expression of RAGE may indicate the existence of severe pathophysiological condition in lung, e.g. acute lung injury (ALI) and acute respiratory distress syndrome (ARDS). During pulmonary tissue injury an endogenous secretory isoform of RAGE called EsRAGE is noticed at high levels in broncho-alveolar lavage (BAL) and plasma. Recently, a soluble form of RAGE (sRAGE) produced by recombinant gene technology was shown to exhibit a therapeutic potential in experimental animal models. Detailed study of RAGE in the pulmonary tissues will facilitate the understanding of the importance of RAGE signaling in the pulmonary health and pathophysiology. © 2008 Elsevier B.V. All rights reserved.

KEYWORDS: advanced glycation end product receptor; bleomycin, article; cell differentiation; cell proliferation; cystic fibrosis; gene technology; human; lung alveolus; lung alveolus epithelium; lung disease; lung function; lung injury; lung metastasis; lung parenchyma; lung transplantation; nonhuman; pathophysiology; priority journal; protein expression; signal transduction, Humans; Lung; Lung Diseases; Receptors, Immunologic

http://www.sciencedirect.com/science/article/pii/S156990480800178X

http://dx.doi.org/10.1016/j.resp.2008.07.001

13. **Deep Jagdeep, S.**, Sidhu Sukhjeet **((2008)** *Methylation pattern of E-cadherin gene as epigenetic biomarker in lung cancer patients.* **Research Journal of Biotechnology, 3 (4), pp. 32-34.**

ABSTRACT: Silencing of tumor suppressor and tumor-related genes by hypermethylation at promoter CpG islands is one of the major events in human tumorigenesis. In this study the methylation pattern of E-cadherin gene was studied in 25 lung cancer patients which included active, passive as well as subjects who had left smoking. The results signify that the methylation pattern can be designated as epigenetic biomarker in lung cancer patients where the diagnosis is not well defined in the early stages of tumorigenesis.

KEYWORDS: Biomaker; CpG islands; E-cadherin; Methylation

www.shankargargh.net/biotek_back_issue/biotek_2008_4/6.pdf

14. Dinesh Khurana., Greg Marks ., Ashish K Srivastava **(2008)** *On Unit-central rings* appear in **the proceedings of conference on Algebra and its application**. **Ohio University., June 18-21.**

Pl also see*: *Advances in ring Theory Trenads in Mathematics (2010) pp.,205-212

ABSTRACT : We establish commutativity theorems for certain classes of rings in which every invertible element is central, or, more generally, in which all invertible elements commute with one another. We prove that if R is a semiexchange ring (i.e. its factor ring modulo its Jacobson radical is an exchange ring) with all invertible elements central, then R is commutative. We also prove that if R is a semiexchange ring in which all invertible elements com- mute with one another, and R has no factor ring with two elements, then R is commutative. We offer some examples of noncommutative rings in which all invertible elements commute with one another, or are central. We close with a list of problems for further research.

KEYWORDS : Exchange rings, Semi-exchange rings, unit-central rings.

link.springer.com/chapter/10.1007%2F978-3-0346-0286-0_13

math.slu.edu/~srivastava/unit-central.pdf

15. Sanjeev Kumar Chandrayan., **Purnananda Guptasarma (2008)** *Partial destabilization of native structure by a combination of heat and denaturant facilitates cold denaturation in a hyperthermophile protein .* **Proteins: Structure, Function and Genetics, 72 (2), pp. 539-546.**

ABSTRACT: Cold denaturation is a phenomenon seen in many different proteins. However, there have been no reports so far of its occurrence in hyperthermophile proteins. Here, using a recombinant triosephosphate isomerase (PfuTIM) from the hyperthermophile archaeon, Pyrococcus furiosus, we show that the heating of this protein through the low temperature side of its thermal unfolding transition in the presence of guanidinium hydrochloride (GdmCl) results in the formation of partially-disordered conformational ensembles that retain considerable native-like secondary and tertiary structure. Unlike PfuTIM itself, these thermochemically obtained partially-disordered PfuTIM ensembles display cold denaturation as they are cooled to room temperature. The protein thus shows hysteresis, adopting different structural states in a manner dependent upon the nature of the heating and cooling treatment, rather than upon the initial and final conditions of temperature and GdmCl concentration, indicating that some sort of a kinetic effect influences structure adoption and retention. The structure lost through cooling of partially-disordered PfuTIM is found to be regained through heating. The ability of GdmCl to thus apparently destabilize the highly thermodynamically and kinetically stable structure of PfuTIM (sufficiently, to cause it to display observable cold-denaturation and heat-renaturation transitions, in real-time, with cooling and heating) offers support to current ideas concerning the how hyperthermophile proteins achieve their high kinetic stabilities, and suggests that desolvation-solvation barriers may be responsible for high kinetic stability. © 2008 Wiley-Liss, Inc.

KEYWORDS: guanidine; recombinant enzyme; triosephosphate isomerase, article; circular dichroism; cold denaturation; cooling; enzyme denaturation; fluorescence spectroscopy; heating; hysteresis; nonhuman; priority journal; protein stability; Pyrococcus furiosus, Archaeal Proteins;Circular Dichroism; Cold; Guanidine; Heat; Kinetics; Protein Conformation; Protein Denaturation; Pyrococcus furiosus; Recombinant Proteins; Spectrometry, Fluorescence; Spectrophotometry, Ultraviolet, Archaea; Pyrococcus furiosus

http://onlinelibrary.wiley.com/doi/10.1002/prot.22077/abstract

DOI: 10.1002/prot.22077

16. Kavita Dorai (**2008**) . Book Review " *Quantum Computing Back Action 2006*, AIP Conference proceedings Vol. 864. Debabrata Goswami (ed.,) **Current Science Vol. 94 (3) pp. 392-393**

http://www.currentscience.ac.in/Downloads/download_pdf.php?titleid=id_094_03_0392_0393_0

17. Divya Kapoor., Vijay Kumar., Sanjeev K., Chandrayan, Shubbir Ahmed, Swati Sharma., Manish Datt., Balvinder Singh., Subramanian Karthikeyan., **Purnananda Guptasarma** (**2008**) *Replacement of the active surface of a thermophile protein by that of a homologous mesophile protein through structure-guided 'protein surface grafting'* . **Biochimica et Biophysica Acta - Proteins and Proteomics, 1784 (11), pp. 1771-1776.**

ABSTRACT: Using several tens of rationally-selected substitutions, insertions and deletions of predominantly non-contiguous residues, we have remodeled the solvent-exposed face of a beta sheet functioning as the substrate-binding and catalytically-active groove of a thermophile cellulase (Rhodothermus marinus Cel12A) to cause it to resemble, both in its structure and function, the equivalent groove of a mesophile homolog (Trichoderma reesei Cel12A). The engineered protein, a mesoactive-thermostable cellulase (MT Cel12A) displays the temperature of optimal function of its mesophile ancestor and the temperature of melting of its thermophile ancestor, suggesting that such 'grafting' of a mesophile-derived surface onto a thermophile-derived structural scaffold can potentially help generate novel enzymes that recombine structural and functional features of homologous proteins sourced from different domains of life. © 2008 Elsevier B.V. All rights reserved.

KEYWORDS: bacterial protein; cellulase; fungal protein; scaffold protein, amino acid sequence; article; cell surface; conformation; enzyme activity; melting point; mesophile; nonhuman; priority journal; protein analysis; protein engineering; protein expression; protein function; protein stability; protein structure; Rhodothermus; sequence alignment; thermophile; thermostability; Trichoderma reesei, Amino Acid Sequence; Catalytic Domain; Cellulases; Hydrogen-Ion Concentration; Models, Molecular; Molecular Sequence Data; Protein

Denaturation; Protein Engineering; Protein Folding; Protein Structure, Secondary; Rhodothermus; Structural Homology, Protein; Surface Properties; Temperature; Thermodynamics; Transition Temperature; Trichoderma, Hypocrea jecorina; Rhodothermus marinus

http://www.sciencedirect.com/science/article/pii/S1570963908001684

http://dx.doi.org/10.1016/j.bbapap.2008.05.007,

18. M.Elango., V.Subramanian.**, N.Sathyamurthy (2008)** *The self-assembly of metaboric acid molecules into bowls, balls and sheets*. **Journal of Physical Chemistry A, 112 (35), pp. 8107-8115.**

ABSTRACT: The structural motifs responsible for the formation of bowls, balls and sheets of orthoboric acid were pointed out in an earlier publication (Elango et al. J. Phys. Chem. A 2005, 109, 8587). It is shown in the present study that metaboric acid forms similar bowls, balls and sheets, despite the fact that the basic unit for cluster formation is different. © 2008 American Chemical Society.

KEYWORDS: Chlorine compounds, Cluster formations; Metaboric acid; Self-assemblies; Structural motifs, Self assembly

http://pubs.acs.org/doi/abs/10.1021/jp8019254

DOI:10.1021/jp8019254

19. M.Elango., V.Subramanian., Anuja P.Rahalkar., Shridhar R.Gadre., **N. Sathyamurthy (2008)** *Structure, energetics, and reactivity of boric acid nanotubes: A molecular tailoring approach* .**Journal of Physical Chemistry A, 112 (33), pp. 7699-7704.**

ABSTRACT: Cardinality guided molecular tailoring approach (CG-MTA) [Ganesh et al. J. Chem. Phys. 2006,125, 104019] has been effectively employed to perform ab initio calculations for large molecular clusters of boric acid. It is evident from the results that boric acid forms nanotubes, structurally similar to carbon nanotubes, with the help of an extensive hydrogen-bonding (H-bonding) network. Planar rosette-shaped hexamer of boric acid is the smallest repeating unit in such nanotubes. The stability of these tubes increases due to enhancement in the number of H-bonding interactions as the diameter increases. An analysis of molecular electrostatic potential (MESP) of these systems provides interesting features regarding the reactivity of these tubes. It is predicted that due to alternate negative and positive potentials on O and B atoms, respectively, boric acid nanotubes will interact favorably with polar systems such as water and can also form multiwalled tubes. © 2008 American Chemical Society.

KEYWORDS: Acids; Boride coatings; Chlorine compounds; Computer networks; Hydrogen; Inorganic acids; Molecular interactions; Nanopores; Nanostructured materials; Nanostructures; Nanotubes; Tubes (components), Boric acids, Carbon nanotubes.

http://pubs.acs.org/doi/abs/10.1021/jp802723e

DOI:10.1021/jp802723e

20. Ravi Chand Singh., Onkar Singh., Manmeet Pal Singh.,**Paramdeep Singh Chandi ((2008)** *Synthesis of zinc oxide nanorods and nanoparticles by chemical route and their comparative study as ethanol sensors* . **Sensors and Actuators, B: Chemical, 135 (1), pp. 352-357. ABSTRACT:** A comparative study of sensing response of zinc oxide nanoparticles and nanorods to ethanol vapours has been reported in this paper. Zinc oxide powder has been synthesized as nanoparticles and nanorods by following a chemical route. The reaction temperature is found to be playing a critical role in the selective synthesis of morphologically distinct nanostructures. Synthesized zinc oxide powder was characterized by using TEM and XRD techniques. Zinc oxide samples were deposited as thick films to act as gas sensors and their comparative response to ethanol vapours was investigated at different temperatures and concentrations. In this work the effect of sintering temperature on the particle size and sensor sensitivity was also studied. The studies revealed that particle size increases with the sintering temperature while sensitivity decreases. The investigations

also revealed that sensing response of ZnO nanoparticles is exceptionally higher than that of ZnO nanorods. © 2008 Elsevier B.V. All rights reserved.

KEYWORDS: Ethanol; Grain size and shape; Nanoparticles; Nanorods; Nanostructured materials; Oxide films; Oxides; Particle size; Powders; Semiconducting zinc compounds; Sensors; Sintering; Synthesis (chemical); Thick films; Vapors; Zinc; Zinc alloys; Zinc oxide, Chemical routes; Comparative studies; Ethanol sensors; Ethanol vapours; Gas sensors; Oxide samples; Reaction temperatures; Selective synthesis; Sensor sensitivities; Sintering temperatures; Synthesis of; Zinc oxide nanoparticles; Zinc oxide nanorods; Zinc oxide powders; ZnO nanoparticles; ZnO Nanorods, Nanostructures.

http://www.sciencedirect.com/science/article/pii/S0925400508005959
http://dx.doi.org/10.1016/j.snb.2008.09.004,

Titles
A - Z : 2009

2009

21. Arvind (2009) *Continuous variable systems: Entanglement, decoherence and quantum cryptography .* **Journal of the Indian Institute of Science, 89 (3), pp. 283-294.**

ABSTRACT: This article aims to review some aspects of quantum information processing (QIP) using continuous variable systems for one and two-modes. The objective of the article is to convey a flavor of the kind of developments which has taken place in this subfield of QIP in the past decade and not to write a comprehensive review of the field. We hence focus on Gaussian states, their entanglement and their utilization in various quantum cryptographic protocols that have been proposed and recently implemented.

KEYWORDS: Continuous variable system; Decoherence; Gaussian state; Of quantum-information; Quantum-cryptographic protocols, Data processing; Quantum cryptography; Quantum optics, Quantum entanglement.

journal.library.iisc.ernet.in/vol200903/Arvind.pdf

22. M.Harti., R.Mikhailov., I.**B.S. Passi., (2009)** Dimensions quotients. **Journal of Indian math. Soc. Special Centenary Vol.(1907-2007)pp.63-107.**

ABSTARCT : We present two approaches , one homological and the other simplicial for the investigation of dimension quotient of groups.The theory is illistrated , in a particular , with a conceptual discussion of fourth and fifth dimension quotient.

http://arxiv.org/pdf/0803.3290.pdf

23. Singh Jagdeep (Editorial Message) (2009) *DNA methylation to Epigenetics molecular Diagnostics.* **Research journal of Biotechnology ., 4(4).**

http://www.biotekjournal.net/back_issue/editorial_Nov%202009.htm

24. C.N.Ramachandran., Dario De Fazio.**, N.Sathyamurthy.**, V.Aquilanti **(2009)** *Guest species trapped inside carbon nanotubes* . **Chemical Physics Letters, 473 (1-3), pp. 146-150.**

ABSTRACT: Taking the torsional motion of H_2O_2 inside a carbon nanotube as an example, the interaction between the encapsulated guest species and the carbon nanotube has been studied using the density functional theoretical method with the B3LYP functional and the 6-31G ** basis set. Depending upon its orientation inside the nanotube, H_2O_2 binds differently with the nanotube thereby inhibiting the torsional motion in the encapsulated state. The binding of the guest species with the nanotube due to the weak O-H···π interaction is discussed. The polarization of the nanotube because of the guest species suggests that the molecular motion through the nanotube may be influenced by polar solvents and external electric fields. © 2009 Elsevier B.V. All rights reserved.

KEYWORDS: Basis sets; Density functional; External electric fields; Guest species; Molecular motions; Polar solvents; Torsional motions, Electric fields, Carbon nanotubes

http://www.sciencedirect.com/science/article/pii/S000926140900390X

http://dx.doi.org/10.1016/j.cplett.2009.03.068

25. Ashwani Kumar Tiwari., Sujitha Kolakkandy.**, N. Sathyamurthy (2009)** *Importance of coriolis coupling in isotopic branching in (He, HD$^+$) collisions.* **Journal of Physical Chemistry A, 113 (34), pp. 9568-9574.**

ABSTRACT: A three-dimensional time-dependent quantum mechanical wave packet approach is used to calculate the reaction probability (P R) and integral reaction cross section values for both channels of the reaction He + HD $^+$(v = 1;j = 0) -- HeH (D) $_+$ + D (H) over a range of translational energy (E trans) on the McLaughlin-ThompsonJoseph- Sathyamurthy potential energy surface including the Coriolis coupling (CC) term in the Hamiltonian. The reaction probability plots as a function of translational energy for different J values exhibit several oscillations, which are characteristic of the system. The σ R values obtained by including CC and not including it are nearly the same over the range of E trans investigated for the HeD$_+$ channel. For the HeH $_+$ channel, on the other hand, σ $_R$ values obtained from CC calculations are significantly smaller than those obtained from coupled state calculations. These results are compared with the available experimental results. The computed branching ratios (T = σ ^{R}(HeH $^+$) / σ ^{R}(HeD $^{+)}$) are also compared with the available experimental results. © 2009 American Chemical Society.

KEYWORDS: Branching ratio; Coriolis coupling; Coupled state; J value; Quantum mechanical; Reaction cross-sections; Reaction probability; Time-dependent; Translational energy; Wave-packet approach, Potential energy; Potential energy surfaces; Quantum chemistry, Helium

http://www.ncbi.nlm.nih.gov/pubmed/19642652

http://pubs.acs.org/doi/abs/10.1021/jp9049523

DOI:10.1021/jp9049523

26. Ravi Chand Singh., Manmeet Pal Singh., Onkar Singh., **Paramdeep Singh Chandi (2009)** *Influence of synthesis and calcination temperatures on particle size and ethanol sensing behaviour of chemically synthesized SnO$_2$ nanostructures* .**Sensors and Actuators, B: Chemical, 143 (1), pp. 226-232.**

ABSTRACT: Nanoparticles of SnO$_2$ have been synthesized through chemical route at 5, 25 and 50 °C. In this work the synthesized particles were calcined at 400, 600 and 800 °C and their structural and morphological analysis was carried out using X-ray diffraction and transmission electron microscopy. The reaction

temperature has been found to be playing a critical role in controlling nanostructure sizes as well as agglomeration. It has been observed that particles synthesized at 5 and 50 °C were smaller and less agglomerated as compared to the particles prepared at 25 °C. The study also reveals that particle size and agglomeration increases with increase in calcination temperature. Thick film gas sensors were fabricated using synthesized tin dioxide powder, and sensing response of all the sensors to ethanol vapours was investigated at different temperatures. The investigations reveal that sensing response of SnO_2 nanoparticles is size dependent and smaller particles are highly sensitive. © 2009 Elsevier B.V. All rights reserved.

KEYWORDS: Calcination temperature; Chemical routes; Ethanol sensing; Ethanol vapours; Gas sensors; Highly sensitive; Morphological analysis; Nanostructure size; Reaction temperature; Sensing response; Size dependent; Synthesized particles, Agglomeration; Calcination; Chemical sensors; Ethanol; Nanoparticles; Thick films; Tin; Tin dioxide; Transmission electron microscopy; X ray diffraction analysis, Synthesis (chemical)

http://www.sciencedirect.com/science/article/pii/S0925400509007357

http://dx.doi.org/10.1016/j.snb.2009.09.032

27. Sébastien Guenneau., **S. Anantha Ramakrishna (2009**) *Negitive refractive index, perfect lenses and checkerboards : Trapping and imaging effects in folded optical spaces*,**Comptes Rendus Physique 10 (5,) PP., 352–378**

ABSTRACT: Newly discovered metamaterials have opened new vistas for better control of light via negative refraction, whereby light refracts in the “wrong” manner. These are dielectric and metallic composite materials structured at subwavelength lengthscales. Their building blocks consist of local resonators such as conducting thin bars and split rings driving the material parameters such as the dielectric permittivity and magnetic permeability to negative (complex) values. Combined together, these structural elements can bring about a (complex valued) negative effective refractive index for the Snell–Descartes law and result in negative refraction of radiation. Negative refractive index materials can support a host of surface plasmon states for both polarizations of light. This

makes possible unique effects such as imaging with subwavelength image resolution through the Pendry–Veselago slab lens. Other geometries have also been investigated, such as cylindrical or spherical lenses that enable a magnification of images with subwavelength resolution. Superlenses of three-fold (equilateral triangle), four-fold (square) and six-fold (hexagonal) geometry allow for multiple images, respectively two, three, and five. Generalization to rectangular and triangular checkerboards consisting of alternating cells of positive and negative refractive index represents a very singular situation in which the density of modes diverges at the corners, with an infinity of images. Sine-cosecant anisotropic heterogeneous square and triangular checkerboards can be respectively mapped onto three-dimensional cubic and icosahedral corner lenses consisting of alternating positive and negative refractive regions. All such systems with corners between negative and positive refractive media display very singular behavior with the local density of states becoming infinitely large at the corner, in the limit of no dissipation. We investigate all of these, using the unifying viewpoint of transformation optics.

http://www.sciencedirect.com/science/article/pii/S163107050900070X

http://dx.doi.org/10.1016/j.crhy.2009.04.002

28. Ramandeep S. Johal (2009) *Quantum heat engines and nonequilibrium temperature* .**Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 80 (4), art. no. 041119,** .

ABSTRACT: A pair of two-level systems initially prepared in different thermal states and coupled to an external reversible work source do not in general reach a common temperature at the end of a unitary work extraction process. We define an effective temperature for the final nonequilibrium but passive state of the bipartite quantum system and analyze its properties. © 2009 The American Physical Society.

KEYWORDS: Bipartite quantum systems; Effective temperature; Non equilibrium; Nonequilibrium temperatures; Quantum heat engines; Reversible work; Thermal state; Two-level system; Work extraction, Quantum electronics; Quantum optics, Heat engines

http://pre.aps.org/abstract/PRE/v80/i4/e041119

DOI: 10.1103/PhysRevE.80.041119

29. Murali, K., Rajamohamed, I., **Sinha, Sudeshna.**, Ditto, William.L., Bulsara, Adi R. **(2009)** *Realization of reliable and flexible logic gates using noisy nonlinear circuits* . **Applied Physics Letters, 95 (19), art. no. 194102, .**

ABSTRACT: It was shown recently [Murali, Phys. Rev. Lett. 102, 104101 (2009)] that when one presents two square waves as input to a two-state system, the response of the system can produce a logical output (NOR/OR) with a probability controlled by the interplay between the system noise and the nonlinearity (that characterizes the bistable dynamics). One can switch or "morph" the output into another logic operation (NAND/AND) whose probability displays analogous behavior; the switching is accomplished via a controlled symmetry-breaking dc input. Thus, the interplay of nonlinearity and noise yields flexible and reliable logic behavior, and the natural outcome is, effectively, a logic gate. This "logical stochastic resonance" is demonstrated here via a circuit implementation using a linear resistor, a linear capacitor and four CMOS-transistors with a battery to produce a cubiclike nonlinearity. This circuit is simple, robust, and capable of operating in very high frequency regimes; further, its ease of implementation with integrated circuits and nanoelectronic devices should prove very useful in the context of reliable logic gate implementation in the presence of circuit noise. © 2009 American Institute of Physics.

KEYWORDS: Bistable dynamics; Circuit implementation; Circuit noise; Controlled symmetry; Linear resistors; Logic operations; Nanoelectronic devices; Non-Linearity; Nonlinear circuit; Square waves; Stochastic resonances; System noise; Two-state systems; Very high frequency, Integrated circuits; Logic gates; Probabilistic logics; Resonance, Logic circuits

http://repository.ias.ac.in/60939/

http://apl.aip.org/resource/1/applab/v95/i19/p194102_s1

Doi:10.1063/1.3245318

30. G.S.S.Saini., Amit Sharma., Sarvpreet Kaur., K.S.Bindra., Vasant Sathe., S.K.Tripathi.**, C.G. Mhahajan** **(2009)** *Rhodamine 6G interaction with solvents studied by vibrational spectroscopy and density functional theory*. **Journal of Molecular Structure, 931 (1-3), pp. 10-19.**

ABSTRACT: We report Raman and infrared spectra of rhodamine 6G dye in different experimental conditions. Positions of some of the observed vibrational bands show noticeable change in the solvents. The bands, which shift, have contributions from the vibrational motion of nitrogen atoms of the ethoxyamine groups, oxygen atom of the ethoxycarbonyl group attached to the phenyl ring and the atoms of the xanthene ring. These shifts arise due to simultaneous interaction of a number of solvent molecules at nitrogen and hydrogen atoms of ethoxyamine, oxygen atom of ethoxycarbonyl and the central oxygen atom of the xanthene ring of the dye molecule. Density functional theory calculations of molecular parameters and atomic charge densities of rhodamine 6G and most probable rhodamine 6G-methanol complexes also support these interactions. Methanol and dimethylformamide also interact electrostatically with the positively charged nitrogen atom of the dye molecule. © 2009 Elsevier B.V. All rights reserved.

KEYWORDS: Density functional theory calculations; Infrared spectra; Raman spectra; Rhodamine 6G; Solvent effect, Atoms; Dimethylformamide; Hydrogen; Infrared spectroscopy; Methanol; Molecules; Nitrogen; Oxygen; Raman scattering; Raman spectroscopy; Solvents; Vibrational spectroscopy, Density functional theory

http://www.sciencedirect.com/science/article/pii/S0022286009002993

http://dx.doi.org/10.1016/j.molstruc.2009.05.015

31. R.N. Gupta., Anjana Khurana., **Dinesh Khurana.**, and T.Y.Lam **(2009)** *Rings over which the transpose of every invertible matrix is invertible*., J**ournal of Algebra 322,(5),, pp. 1627–1636**

Abstract: We prove that the transpose of every invertible square matrix over a ring R is invertible if and only if R/rad(R) is commutative. Many other characterizations are obtained for such rings R in terms of U(R) (the group of units of R), including, for instance, $c+ba \in U(R) \Rightarrow c+ab \in U(R)$, and $1+abc-cba \in U(R)$ (for all $a,b,c \in R$). We also consider a natural weakening of these conditions, namely, $1+abc \in U(R) \Rightarrow 1+cba \in U(R)$, and show that, for von Neumann regular rings, this is a (necessary and) sufficient condition for the commutativity of R.

KEYWORDS : Noncommutative rings; Invertible matrices; Transposes; Jacobson redical; Additive Commutators

http://www.sciencedirect.com/science/article/pii/S0021869309003482

http://dx.doi.org/10.1016/j.jalgebra.2009.05.029

32. Sukhdeep Kumar., Neha Jain., Tapan K.Mukherjee (2009) *Role of RAGE in idiopathic pulmonary fibrosis: Promising prospects*. R**espiratory Physiology and Neurobiology, 165 (2-3), pp. 121-122.**

KEYWORDS: advanced glycation end product receptor; CD40 ligand; messenger RNA, cardiovascular disease; DNA polymorphism; fibrosing alveolitis; kidney disease; letter; lung fibroblast; lung lavage; microalbuminuria; priority journal; retinopathy; risk; RNA splicing

http://www.sciencedirect.com/science/article/pii/S1569904808002954

http://dx.doi.org/10.1016/j.resp.2008.10.018

33. Harpreet K. Grover., **Dinesh Khurana (2009)** *Some characterizations of VNL rings*. **Communications in Algebra, 37 (9), pp. 3288-3305.**

ABSTRACT: A ring R is said to be von Newmann local (VNL) if for any a ∈ R, either a or 1 -a is (von Neumann) regular. The class of VNL rings lies properly between exchange rings and (von Neumann) regular rings. We characterize abelian VNL rings. We also characterize and classify arbitrary VNL rings without an infinite set of orthogonal idempotents; and also the VNL rings having a primitive idempotent e such that eRe is not a division ring. We prove that a semiperfect ring R is VNL if and only if for any right uni-modular row (a1, a2) ∈ R2, one of the ai's is regular in R. Formal triangular matrix rings that are VNL are also characterized. As a corollary, it is shown that an upper triangular matrix ring Tn(R) is VNL if and only if n = 2 or 3 and R is a division ring. © Taylor & Francis Group, LLC.

KEYWORDS: Exchange rings; Semiperfect rings; VNL rings

http://www.tandfonline.com/doi/full/10.1080/00927870802502761

http://arxiv.org/abs/0801.2470

DOI:10.1080/00927870802502761

34. S. Anantha Ramakrishna., Akhlesh Lakhtakia (**2009**) *Spectral shifts in the properties of a periodic multilayered stack due to isotropic chira layers*. **J.Opt. A : Pure Appl.Opt. Vol.11,074001.**

ABSTRACT: Investigating the canonical problem of a periodic multilayered stack containing isotropic chiral layers, we homogenized it as a uniaxial bianisotropic medium and derived its effective constitutive parameters. The stack shows a resonant behavior, when its unit cell consists of a metallic layer and an isotropic chiral layer. The presence of isotropic chirality can result in small shifts of the resonance frequency for reasonably large values of the chirality parameter, implying that the sign of an effective permittivity can be switched. Such spectral shifts in the dielectric properties can be potentially useful for spectroscopic purposes.

KEYWORDS : homogenization, isotropic chirality, negative permittivity, periodic multilayered metamaterial

http://arxiv.org/abs/0902.2094

http://iopscience.iop.org/1464-4258/11/7/074001/

35. R.Parthasarathi., M.Elango., V.Subramanian., **N.Sathyamurthy(2009)** *Structure and stability of water chains* $(H_2O)_n$*, n = 5-20* . **Journal of Physical Chemistry A, 113 (16), pp. 3744-3749.**

ABSTRACT: The structure and stability of linear (helical) water chains $(H_2O)_n$, n = 5-20 as obtained from ab initio/DFT calculations are reported along with an atoms-in-molecules (AIM) analysis of hydrogen bond critical points and their characteristics. The resulting helical chain arrangement is one of the predominant motifs in different host environments; although they may not be the most stable, it is shown that these linear water chain clusters could exist in their own right. © 2009 American Chemical Society.

KEYWORDS: Atoms-in-molecules; Bond critical points; Helical chains, Equations of state; Hydrogen; Hydrogen bonds, Water analysis

http://www.ncbi.nlm.nih.gov/pubmed/19143553

http://pubs.acs.org/doi/abs/10.1021/jp806793e

DOI: 10.1021/jp806793e

36. Ramesh Kapoor., Anand Gupta, Paloth Venugopalan., Ajay Pal Singh Pannu., Maninder Singh Hundal., Pratibha Kapoor **(2009)** *Structural studies of diorganotin(IV) sulfonates: The synthesis of [(n-C_4H_9)$_2$Sn{$OSO_2C_6H_3(CH_3)_2$-2,5}$_2$] and [(n-C_4H_9)$_2$Sn{OSO_2R)$_2$ · 2(hexamethylphosphoric triamide)] [R=CH_3, 4-$C_6H_4CH_3$, 2,5-$C_6H_3(CH_3)_2$] 2,5,6-$C_6H_2(CH_3)_3$] and crystal structures of [(n-C_4H_9)$_2$Sn(μ-OH)($OSO_2C_6H_3(CH_3)_2$-2,5)]$_2$ and (n-C_4H_9)$_2$Sn{OSO_2R)$_2$· 2(hexamethylphosphoric triamide)] [R=4-$C_6H_4CH_3$, 2,5-$C_6H_3(CH_3)_2$, 2,4,6-$C_6H_2(CH_3)_3$].* **Journal of Organometallic Chemistry, 694 (5), pp. 623-629.**

ABSTRACT: The synthesis of [(n-C_4H_9)$_2$Sn{$OSO_2C_6H_3(CH_3)_2$-2,5}$_2$] and [(n-C_4H_9)$_2$Sn{OSO_2R)$_2$ · 2(hexamethylphosphoric triamide)] [R = CH_3 (3), 4-$C_6H_4CH_3$, (4) 2,5-$C_6H_3(CH_3)$ 2 (5), 2,4,6-$C_6H_2(CH_3)_3$ (6) and have been carried out to study their structures and to delineate the coordination behavior of the weakly coordinating sulfonate anions. Compound 1 hydrolyzes slowly to [(n-C_4H_9)$_2$Sn(μ-OH)($OSO_2C_6H_3(CH_3)_2$-2,5)]$_2$ (**2**) when kept in CH_2Cl_2 for a few days. The crystal structure shows that 2 has a dimeric structure in which tin atoms are bridged by two hydroxy groups and each tin atom is further bonded to two *n-Bu* groups and a mono-coordinated sulfonate anion thus generating a trigonal bipyramidal geometry at tin atom. However, the coordination geometry at tin can be visualized as a severely distorted octahedron, if a relatively weak Sn-O bond of 2.690 Å between Sn and an O atom of the neighboring sulfonate anion is also considered. Compounds 3-6 are obtained by the consecutive reaction of (n-C_4H_9)$_2$SnO with the appropriate sulphonic acid and hexamethylphosphoric triamide (HMPA). X-ray crystal structures of 4, 5 and 6 show octahedral geometry around tin atom in the two compounds in which the sulfonate ligands are covalently bonded in a monodentate mode. Compounds 3-6 are nonionic in polar solvents. The Sn-O (sulfonate) bond distances 2.354(2), 2; 2.233(2), 4; 2.237(5), 5 and 2.227(3) Å, 6 suggest some degree of ionic character in the metal-anion bonds. These compounds have also been characterized by multinuclear (^{1}H,^{13}C and^{119}Sn) NMR studies. © 2008 Elsevier B.V. All rights reserved.

KEYWORDS: Atomic physics; Atoms; Complexation; Computational geometry; Coordination reactions; Crystal structure; Ions; Negative ions; Nuclear magnetic resonance; Nuclear magnetic resonance spectroscopy; Organic acids; Self assembly; Synthesis (chemical); Tin; Titanium compounds, Crystal structures; Diorganotin(IV) sulfonate; Hexamethylphosphoric triamide; IR spectra; NMR spectra, Crystal atomic structure

http://www.sciencedirect.com/science/article/pii/S0022328X0800764X
http://dx.doi.org/10.1016/j.jorganchem.2008.11.031

37. M. Elango., V. Subramanian., **N. Sathyamurthy (2009)** *Structure and stability of spiro-cyclic water clusters* . **Journal of Chemical Sciences, 121 (5), pp. 839-848.**

ABSTRACT: The structure and stability of spiro-cyclic water clusters containing up to 32 water molecules have been investigated at different levels of theory. Although there exist minima lower in energy than these spiro-cyclic clusters, calculations at the Hartree-Fock level, density functional theory using B3LYP parametrization and second order Møller-Plesset perturbation theory using 6-31G* and 6-311++G** basis sets show that they are stable in their own right. Vibrational frequency calculations and atoms-in- molecules analysis of the electron density map confirm the robustness of these hydrogen bonded clusters. © Indian Academy of Sciences.

KEYWORDS: Atoms-in-molecules; Atoms-in-molecules analysis; Basis sets; Cyclic clusters; Electron densities; Hartree-Fock levels; Hydrogen bonded clusters; Hydrogen bonding; Parametrizations; Plesset perturbation theory; Second orders; Spiro-cyclic; Vibrational frequencies; Water cluster; Water clusters; Water molecule, Atoms; Hydrogen; Hydrogen bonds; Molecules; Perturbation techniques, Density functional theory

www.ias.ac.in/chemsci/Pdf-Sep2009/839.pdf

38. Debmalya Roy., N.K. Tripathi., K. Ram., **N. Sathyamurthy (2009)** *Synthesis of germanium encapsulated fullerene*. **Solid State Communications, 149 (31-32), pp. 1244-1247.**

ABSTRACT: A method has been described for encapsulating Ge in a fullerene cage using GeO_2 and a graphite composite rod as anode and graphite as cathode. Annealing in an inert atmosphere before arcing, and the amount of GeO_2 in the rod determined the yield of Ge doped metallofullerene. Solvent extraction using soxlet in inert atmosphere followed by calcination in air was used to isolate metallofullerene from the soot. The insertion of Ge inside the fullerene was proven by ultra violet-visible absorption spectroscopy, matrix assisted laser desorption ionization-time of flight mass spectroscopy, Fourier transform infrared spectroscopy, energy-dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy. © 2009 Elsevier Ltd. All rights reserved.

KEYWORDS: A. Fullerenes; D. Quantum localization; E. Atom, molecule and ion impact; Energy dispersive x-ray spectroscopy; Fullerene cages; Graphite composites; Inert atmospheres; Matrix assisted laser desorption ionization; Metallofullerene; Time-of-flight mass spectroscopy; Ultra violet-visible, Atoms; Calcination; Desorption; Fourier transform infrared spectroscopy; Fullerenes; Germanium; Graphite; Ion bombardment; Mass spectrometry; Solvent extraction; Solvents; Spectroscopic analysis; Spectrum analysis; X ray photoelectron spectroscopy, Absorption spectroscopy

http://www.sciencedirect.com/science/article/pii/S0038109809003159

http://dx.doi.org/10.1016/j.ssc.2009.05.039

Titles
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2010

39. S.M. Kamil., Gautam I.Menon., **Sudeshna Sinha (2010)** *A Coupled Map Lattice Model for Rheological Chaos in Sheared Nematic Liquid Crystals,* **Chaos 20, 043123.1 - 043123.14**

ABSTRACT: A variety of complex fluids under shear exhibit complex spatio-temporal behaviour, including what is now termed rheological chaos, at moderate values of the shear rate. Such chaos associated with rheological response occurs in regimes where the Reynolds number is very small. It must thus arise as a consequence of the coupling of the flow to internal structural variables describing the local state of the fluid. We propose a coupled map lattice (CML) model for such complex spatio-temporal behaviour in a passively sheared nematic liquid crystal, using local maps constructed so as to accurately describe the spatially homogeneous case. Such local maps are coupled diffusively to nearest and next nearest neighbours to mimic the effects of spatial gradients in the underlying equations of motion. We investigate the dynamical steady states obtained as parameters in the map and the strength of the spatial coupling are varied, studying local temporal properties at a single site as well as spatio-temporal features of the extended system. Our methods reproduce the full range of spatio-temporal behaviour seen in earlier one-dimensional studies based on partial differential equations. We report results for both the one and two-dimensional cases, showing that spatial coupling favours uniform or periodically time-varying states, as intuitively expected. We demonstrate and characterize regimes of spatio-temporal intermittency out of which chaos develops. Our work suggests that such simplified lattice representations of the spatio-temporal dynamics of complex fluids under shear may provide useful insights as well as fast and numerically tractable alternatives to continuum representations.

http://arxiv.org/abs/1005.2041

http://chaos.aip.org/resource/1/chaoeh/v20/i4/p043123_s1

40. **Rajesh Kochhar** **(2010)** *Ancient Indian astro-mathematical tradition: Evolution and linkages .* **AIP Conference Proceedings, 1283, pp. 156-160.**

ABSTRACT: Indian astronomical tradition is characterized by antiquity, continuity and interaction with the outside world. From 6th century CE till the time of Kepler's laws, Indian astronomers were probably the only ones in the world who could calculate eclipses with any degree of accuracy. In the 12th century, an astronomer in Central India, Padmanabha by name, predicted the lunar eclipse of 8 November 1128 and was rewarded by the king with a land grant (Mirashi 1933-34). The tradition was alive well into the 19th century. By means of shells arranged on the ground and using mathematical tables memorized "by means of certain artificial words and syllables", a "Kalendar maker residing in Pondicherry" calculated the lunar eclipse of 31 May-1 June 1825, with an error of no more than +4 minutes for the beginning (Neugebauer 1983, p. 436). Even now, traditional astronomical almanacs in India, known as panchangas, used in India for ritual and religious purposes base their calculations on ancient texts. It is only in the case of eclipse that they borrow data from modern sources. The beginnings of astronomy are related to the requirements of the ritual in early cultures. Ritual was seen as a means of securing divine approval and support for terrestrial actions. To be effective, it had to be elaborate and welltimed, so that a careful distinction could be made between auspicious and inauspicious times. Since planetary motions provided a natural means of time keeping and were seen as embodiment of divine signals, astronomy developed as an intellectual discipline (see Yano 2003). Similarly mathematics grew as an aid to designing sacrificial altars. The oldest geometry texts in India are the Sulvasutras which dealt with questions like the square root of two. Different scholars place the earlier of these texts anywhere between 800 BCE and 400 BCE. Astronomy texts are decidedly older. Subsequent developments in mathematics came about as an astronomical aid. © 2010 American Institute of Physics.

http://proceedings.aip.org/resource/2/apcpcs/1283/1/156_1?isAuthorized=no

doi:http://dx.doi.org/10.1063/1.3506051

41. B. Sutar., **K. P. Singh.**, V. Bhide., D. Zollman., A.Mody (**2010**) *Application of single-slit diffraction to measure Youngs modulus,* **Lat. Am. J. Phys. Edu. 4, 497**

ABSTRACT : We demonstrate an application of the laser diffraction by a single-slit to measure the Young's modulus of the material of a wire. The standard Searle's apparatus is modified to exploit the sensitivity of the diffraction pattern for changes in slit widths of the order of laser wavelengths produced by micro elongations in the wire when a stress is applied to it. The experiment is performed using different lasers as well as for wires of different materials and produces results with an error of few percent.

KEYWORDS: Young’s modulus, single-slit diffraction, micro-displacement.

http://dialnet.unirioja.es/servlet/articulo?codigo=3696572

www.lajpe.org/sep10/400_Ashok_Mody.pdf

PACS: 01.40.Fk, 06.30.Bp, 07.10.Pz

http://www.journal.lapen.org.mx/sep10/LAJPE_400_Ashok_Mody_preprint_f.pdf

42. Manoj Kumar Pandey., **Ramesh Ramachandran (2010)** *A theoretical perspective on the accuracy of rotational resonance (R 2)-based distance measurements in solid-state NMR* . **Molecular Physics, 108 (5), pp. 619-635.**

ABSTRACT: The application of solid-state NMR methodology for bio-molecular structure determination requires the measurement of constraints in the form of 13_C- 13_C and 13_C- 15_N distances, torsion angles and, in some cases, correlation of the anisotropic interactions. Since the availability of structurally important constraints in the solid state is limited due to lack of sufficient spectral resolution, the accuracy of the measured constraints become vital in studies relating the three-dimensional structure of proteins to its biological functions. Consequently, the theoretical methods employed to quantify the experimental data become important. To accentuate this aspect, we re-examine analytical two-spin models currently employed in the estimation of 13_C- 13_C distances based on the rotational resonance (R 2) phenomenon. Although the error bars for the estimated distances tend to be in the range 0.5-1.0 Å, R 2 experiments are routinely employed in a variety of systems ranging from simple peptides to more complex amyloidogenic proteins. In this article we address this aspect by highlighting the systematic errors introduced by analytical models employing

phenomenological damping terms to describe multi-spin effects. Specifically, the spin dynamics in R 2 experiments is described using Floquet theory employing two different operator formalisms. The systematic errors introduced by the phenomenological damping terms and their limitations are elucidated in two analytical models and analysed by comparing the results with rigorous numerical simulations. © 2010 Taylor & Francis.

KEYWORDS: Analytical model; Anisotropic interaction; Bio-molecular; Biological functions; Error bars; Experimental data; Floquet theory; Numerical simulation; Rotational resonance; Solid state NMR; Spin effects; Spin models; Structure determination; Three-dimensional structure of protein; Torsion angle, Complexation; Computer simulation; Damping; Differential equations; Errors; Experiments; Models; Nuclear magnetic resonance; Nuclear magnetic resonance spectroscopy; Proteins; Resonance; Solid state physics; Systematic errors, Spin dynamics

http://www.tandfonline.com/doi/abs/10.1080/00268971003645347

DOI:10.1080/00268971003645347

43. Kamal P.Singh., Jan M.Rost **(2010)** A*tomic and molecular systems driven by intense random light* . **Chemical Physics, 375 (2-3), pp. 144-149.**

ABSTRACT: We investigate dynamics of atomic and molecular systems exposed to intense, shaped random fields and a weak femtosecond laser pulse theoretically. As a prototype example, the photoionization of a hydrogen atom is considered in detail. The net photoionization undergoes an optimal enhancement when a broadband random field is added to the weak laser pulse. The enhanced ionization is analyzed using time-resolved wavepacket evolution and the population dynamics of the atomic levels. We elucidate the enhancement produced by spectrally shaped random fields of two different classes, one with a tunable bandwidth and another with a narrow bandwidth centered at the first

atomic transition. Motivated by the large bandwidth provided in the high harmonic generation, we also demonstrate the enhancement effect exploiting random fields synthesized from discrete, phase randomized, odd-order and all-order high harmonics of the driving pulse. These findings are generic and can have applications to other atomic and simple molecular systems. © 2010 Elsevier B.V. All rights reserved.

KEYWORDS: Stochastic processes

http://www.sciencedirect.com/science/article/pii/S0301010410003733

http://dx.doi.org/10.1016/j.chemphys.2010.08.003

44. I.B.S.Passi., Mahender Singh., Manoj K. Yadav **(2010)** *Automorphisms of abelian group extensions* . **Journal of Algebra, 324 (4), pp. 820-830.**

ABSTRACT: Let 1 → N→ G→ H→ 1 be an abelian extension. The purpose of this paper is to study the problem of extending automorphisms of N and lifting automorphisms of H to certain automorphisms of G. © 2010 Elsevier Inc. **KEYWORDS**: Automorphisms of groups; Cohomology of groups; Split extensions

http://arxiv.org/abs/0911.4250

http://www.sciencedirect.com/science/article/pii/S0021869310001766

45. William L., Ditto, A.Miliotis., K.Murali., **Sudeshna Sinha,** , Mark L. Spano (2010) *Chaogates: Morphing logic gates that exploit dynamical patterns*. **Chaos, 20 (3), art. no. 037107,** .

ABSTRACT: Chaotic systems can yield a wide variety of patterns. Here we use this feature to generate all possible fundamental logic gate functions. This forms the basis of the design of a dynamical computing device, a chaogate, that can be rapidly morphed to become any desired logic gate. Here we review the basic concepts underlying this and present an extension of the formalism to include asymmetric logic functions. © 2010 American Institute of Physics.

http://chaos.aip.org/resource/1/chaoeh/v20/i3/p037107_s1

http://dx.doi.org/10.1063/1.3489889

46. S.Begam Elavarasi., **Kavita Dorai** **(2010)** *Characterization of the 19 F chemical shielding tensor using cross-correlated spin relaxation measurements and quantum chemical calculations* . **Chemical Physics Letters, 489 (4-6), pp. 248-253.**

ABSTRACT: The 19 F chemical shift anisotropy (CSA) tensor is an indispensable structure estimation tool in the NMR investigations of flourinated biomolecules. This work focuses on the characterization of the 19 F CSA tensor in small molecules, through the combined use of quantum chemical methods and liquid-state NMR cross-correlated spin relaxation experiments. The effect of different basis sets and quantum computational methods on the magnitude and orientation of the 19 F CSA tensor are discussed. The results from ab initio methods and the liquid-state relaxation experiments match well and are comparable to values of the CSA tensor obtained from previous solid-state studies and from theoretical investigations of similar molecules. © 2010 Elsevier B.V. All rights reserved.

KEYWORDS: Ab initio method; Basis sets; Chemical shielding tensors; Chemical shift anisotropy; Flourinated; Liquid state; Quantum cViskahihemical calculations; Quantum-chemical methods; Small molecules; Spin relaxation; Structure estimation; Theoretical investigations; Work Focus, Electric currents; Experiments; Liquids; Nuclear magnetic resonance; Quantum chemistry; Quantum theory; Spin dynamics; Tensors, Chemical shift

http://www.sciencedirect.com/science/article/pii/S0009261410002733

http://dx.doi.org/10.1016/j.cplett.2010.02.078

47. Sudeshna Sinha **(2010)** *Clipping Chaos to Cycles:* invited Chapter in the book **Recent progress in controlloing chaos,** Editor :C.Grebogi and M.A.F. Sanjuan (World scienctifc)pp. 239-266

http://www.worldscientific.com/doi/abs/10.1142/9789814291705_0008

doi: 10.1142/9789814291705_0008

48. Mohamed, I.Raja., Murali, K., **Sinha, Sudeshna**., Lindberg, Eric (**2010)** *Design of threshold controller based chaotic circuits*. **International Journal of Bifurcation and Chaos, 20 (7), pp. 2185-2191.**

ABSTRACT: We propose a very simple implementation of a second-order nonautonomous chaotic oscillator, using a threshold controller as the only source of nonlinearity. We demonstrate the efficacy and simplicity of our design through numerical and experimental results. Further, we show that this approach of using a threshold controller as a nonlinear element, can be extended to obtain autonomous and multiscroll chaotic attractor circuits as well. © 2010 World Scientific Publishing Company.

KEYWORDS: bifurcation; Chaos; Chaotic circuits; Chaotic oscillators; Multiscroll chaotic attractor; Non-Linearity; Nonautonomous; Nonlinear elements; Second orders; threshold controller, Bifurcation (mathematics); Circuit oscillations; Networks (circuits), Controllers

http://www.dtu.dk/centre/ele/English/about_us/staff.aspx?lg=showcommon&id=83de7254-3a91-4f16-b424-ddb7d9652d13

10.1142/S0218127410027015

49. Rajesh Kochhar (2010) *Engineering vis-à-vis science: India's missed discovery of water on the moon* . Current Science, 98 (12), pp. 1549-1550.

http://cat.inist.fr/?aModele=afficheN&cpsidt=23638033

http://www.currentscience.ac.in/Downloads/article_id_098_12_1549_1550_0.pdf

50. Ravi Chand Singh., Manmeet Pal Singh., Onkar Singh., **Paramdeep Singh Chandi**, Ravi Kumar **(2010)** *Effect of 100 MeV O* 7_{+} *ions irradiation on ethanol sensing response of nanostructures of ZnO and SnO* ^{2} . **Applied Physics A: Materials Science and Processing, 98 (1), pp. 161-166.**

ABSTRACT: Tin dioxide nanoparticles and zinc oxide nanorods were synthesized chemically and thick film gas sensors on alumina substrates were fabricated of these materials. Morphology and crystallite size of synthesized powders were investigated by TEM. The fabricated sensors were irradiated with 100 MeV O 7$_{+}$ ions at fluences of 1×10 $_{11}$, 1×10 $_{12}$ and 1×10 $_{13}$ ions/cm $_{2.}$ The X-ray diffraction analysis of the samples before and after ion bombardment was performed for structural characterization. The sensing response to ethanol before and after irradiation was carried out for each fabricated sensor. Investigation revealed that irradiated SnO^{2} based sensor's response and response time increased significantly. Results show that ZnO based sensor exhibit strong resistance to damage caused by ion irradiation which might be due to defects annihilation. © 2009 Springer-Verlag.

KEYWORDS: Alumina substrates; Before and after; Ethanol sensing; Fabricated sensors; Fluences; Gas sensors; Ion irradiation; Ions irradiation; Response time; Sensing response; Structural characterization; Synthesized powder; TEM; Tin dioxide nanoparticles; Zinc oxide nanorods; ZnO; ZnO and SnO, Crystallite size; Ethanol; Fabrication; Ion bombardment; Ions; Nanorods; Semiconducting zinc compounds; Sensors; Thick films; Tin; Tin dioxide; Zinc; Zinc oxide, X ray diffraction analysis

http://link.springer.com/article/10.1007%2Fs00339-009-5442-5?LI=true#page-1

*DOI 10.1007/s00339-009-5442-*5

51. Pratibha Kapoor., Ajay Pal Singh Pannu., Geeta Hundal., **Ramesh Kapoor.**, Montserrat Corbella., Núria Aliaga-Alcalde., Maninder Singh Hundal **(2010)** *First report on N,N′-diisoalkylisonicotinamide 1D coordination network containing linear trinuclear [CO$_3$L$_4$Cl$_6$] units with mixed Co^{II}(T$_d$)-Co^{II}(O$_h$)-Co^{II}(T$_d$) geometries: Structure and magnetic properties*.**Dalton Transactions, 39 (34), pp. 7951-7959.**

ABSTRACT: Reaction of anhydrous CoCl$_2$ with N,N′- diisopropylisonicotinamide (L) has yielded a coordination polymer containing linear trinuclear [Co$_3$L$_4$Cl$_6$] units with a rare, mixed Co(T$_d$)-Co(O$_h$)-Co(T$_d$) assembly (compound 1). The central Co^{II} ion, of each trinuclear entity, exhibits a distorted octahedral

geometry, with two ligand molecules coordinating through their carbonyl oxygen atoms along with two bridging Cl^- ions and two pyridine N atoms from the neighboring molecules. Also, in each unit, two outer Co^{II} ions display distorted tetrahedral geometry, coordinating to one ligand molecule through the pyridine N atom and to three Cl^- ions (one of them bridged to the central Co^{II} and the two acting as a terminal ligands). The magnetic properties of this compound were investigated in the temperature range of 2.0 to 300.0 K. Owing to the complexity of the system and the weak interactions among trinuclear aggregates, the magnetic response has been analyzed using a model which considers these units as isolated systems. In addition, magnetic data has been examined in two separated blocks, above and below 50 K, applying programs VPMAG FORTRAN and MAGPACK-fit, respectively. This way, only the most significant effects at each interval of temperature were considered: spin-orbit coupling of the $Co(O^h)$, at high temperatures and zero-field splitting parameters of the $Co(T_d)$ at the low. Spin-spin magnetic interaction has been taken into account for the whole range of temperatures. As a result, the analysis of the magnetic data shows that, within every trinuclear unit, the central position matches well with a high-spin Co^{II} (S = 3/2) and also reveals weak ferromagnetic interactions between the $Co(O_h)$ and the two terminal $Co(T_d)$ ions ($J = +0.34$ cm^-1). © 2010 The Royal Society of Chemistry.

KEYWORDS: Carbonyl oxygen atoms; Coordination networks; Coordination Polymers; Ferro-magnetic interactions; Fortran; High temperature; Isolated systems; Ligand molecules; Magnetic data; Magnetic interactions; Magnetic response; Neighboring molecules; Octahedral geometry; Spin-orbit couplings; Spin-spin; Temperature range; Terminal ligands; Tetrahedral geometry; Weak interactions; Zero-field splitting parameters, Atoms; Geometry; Ions; Ligands; Magnetic properties; Magnetic storage; Molecules; Oxygen; Pyridine, Magnetism

http://www.ncbi.nlm.nih.gov/pubmed/20657942

http://pubs.rsc.org/en/Content/ArticleLanding/2010/DT/c0dt00245c

DOI:10.1039/C0DT00245C

52. A. Kenfack., **K.P. Singh (2010)** *From Physics to control through an emergent view,* **World Scientific, Series B, vol.15, 63-68**

The book is a compilation of selected papers from the conference on *Physics and Control 2009*, presenting a unified perspective underlying the thematics and strategies related to the control of physical systems with emerging applications in physics, engineering, chemistry, biology and other natural sciences. The selected papers reflect the state-of-the-art of the more advanced theoretical and practical studies in the field of control of complex systems. The contributions provide a comprehensive view on some selected topics of particular importance at the disciplinary borderline between Physics and Control.

http://www.worldscientific.com/doi/abs/10.1142/9789814313155_0010

doi: 10.1142/9789814313155_0010

53. James P. Crutchfield., William L. Ditto.**, Sudeshna Sinha (2010)** *Introduction to focus issue: Intrinsic and designed computation: Information processing in dynamical systems-beyond the digital hegemony*. **Chaos, 20 (3), Art. No. 037101**.

ABSTRACT: How dynamical systems store and process information is a fundamental question that touches a remarkably wide set of contemporary issues: from the breakdown of Moore's scaling laws-that predicted the inexorable improvement in digital circuitry-to basic philosophical problems of pattern in the natural world. It is a question that also returns one to the earliest days of the foundations of dynamical systems theory, probability theory, mathematical logic, communication theory, and theoretical computer science. We introduce the broad and rather eclectic set of articles in this Focus Issue that highlights a range of current challenges in computing and dynamical systems. © 2010 American Institute of Physics.

http://chaos.aip.org/resource/1/chaoeh/v20/i3/p037101_s1

http://dx.doi.org/10.1063/1.3492712

54. Ville Keranen., Esko Keski-Vakkuri., Sean Nowling., **K. P. Yogendran (2010)** I*nho-mogeneous structures in holographic superfluids. I. Dark solitons.,* **Phys. Rev. D 81, 126011**

ABSTRACT: We begin an investigation of inhomogeneous structures in holographic superfluids. As a first example, we study domain wall-like defects in the 3+1 dimensional Einstein-Maxwell-Higgs theory, which was developed as a dual model for a holographic superconductor. In [V. Keränen, E. Keski-Vakkuri, S. Nowling and K. P. Yogendran Phys. Rev. D **80** 121901 (2009)], we reported on such "dark solitons" in holographic superfluids. In this work, we present an extensive numerical study of their properties, working in the probe limit. We construct dark solitons for two possible condensing operators and find that both of them share common features with their standard superfluid counterparts. However, both are characterized by two distinct coherence length scales (one for order parameter, one for charge condensate). We study the relative charge depletion factor and find that solitons in the two different condensates have very distinct depletion characteristics.

http://prd.aps.org/abstract/PRD/v81/i12/e126011

DOI: 10.1103/PhysRevD.81.126011

55. Ville Keranen., Esko Keski-Vakkuri., Sean Nowling., **K. P. Yogendran (2010)** I*nho-mogeneous structures in holographic superfluids. II. Vortices.* **Phys. Rev. D 81,126012**

ABSTRACT : We study vortex solutions in a holographic model of Herzog, Hartnoll, and Horowitz, with a vanishing external magnetic field on the boundary, as is appropriate for vortices in a superfluid. We study the relevant length scales related to the vortices and how the charge density inside the vortex core behaves as a function of temperature or chemical potential. We extract a critical superfluid velocity from the vortex solutions, study how it behaves as a function of the temperature, and compare it to earlier studies and to the Landau criterion. We also comment on the possibility of a Berezinskii-Kosterlitz-Thouless vortex confinement-deconfinement transition.

http://prd.aps.org/abstract/PRD/v81/i12/e126012

DOI: 10.1103/PhysRevD.81.126012

56. Roman Mikhailov., **Inder Bir S. Passi (2010)** *Limits over categories of extensions* .**Indian Journal of Pure and Applied Mathematics, 41 (1), pp. 113-131.**

ABSTRACT: We consider limits over categories of extensions and show how certain well-known functors on the category of groups turn out as such limits. We also discuss higher (or derived) limits over categories of extensions. © Indian National Science Academy.

KEYWORDS: Categories of extensions; Derived functors; Divided power functors; Functors; Higher limits; Inverse limit; Symmetric power; Tensor power

http://link.springer.com/article/10.1007%2Fs13226-010-0012-2?LI=true#page-1

57. Adi R.Bulsara., Anna Dari., William L.Ditto., K.Murali., **Sudeshna Sinha (2010)** *Logical stochastic resonance.* **Chemical Physics, 375 (2-3), pp. 424-434.**

ABSTRACT: In a recent publication it was shown that, when one drives a two-state system with two square waves as input, the response of the system mirrors a logical output (NOR/OR). The probability of obtaining the correct logic response is controlled by the interplay between the noise-floor and the nonlinearity. As one increases the noise intensity, the probability of the output reflecting a NOR/OR operation increases to unity and then decreases. Varying the nonlinearity (or the thresholds) of the system allows one to morph the output into another logic operation (NAND/AND) whose probability displays analogous behavior. Thus, the outcome of the interplay of nonlinearity and noise is a flexible logic gate with enhanced performance. Here we review this concept of "Logical Stochastic Resonance" (LSR) and provide details of an electronic circuit system demonstrating LSR. Our proof-of-principle experiment involves a particularly simple realization of a two-state system realized by two adjustable thresholds. We also review CMOS implementations of a simple LSR circuit, and the concatenation of these LSR modules to emulate combinational logic, such as data flip-flop and full adder operations. © 2010 Elsevier B.V. All rights reserved.

KEYWORDS: Logic gates; Stochastic resonance

http://www.sciencedirect.com/science/article/pii/S0301010410002831

http://dx.doi.org/10.1016/j.chemphys.2010.06.015

58. S. Begam Elavarasi., **Kavita Dorai** (**2010)** *Mapping NMR chemical shift anisotropy parameters of backbone nuclei onto secondary structure elements in proteins*. **Journal of Biomolecular Structure and Dynamics, 27 (4), pp. 561-572.**

ABSTRACT: There has been much recent progress in using NMR chemical shift anisotropy (CSA) parameters to gain information about secondary structure content in proteins. This paper focuses on the comparison of CSA tensors of different backbone nuclei (namely $^{13}C^{a}$, $^{13}C'$, ^{15}N,$^{1}H^{a}$, $^{1}H^{N}$) of all twenty amino acids appearing in well-defined secondary structures such as helices and sheets. Dihedral angle information of these backbone nuclei in different secondary structure elements has been extracted from experimentally determined structures of proteins deposited in the protein databank. The CSA tensors of these backbone nuclei have been computed for the corresponding dihedral angles using ab initio quantum chemical methods. It is shown that 2D correlated plots of a novel set of CSA parameters (ρ,τ), that define the magnitude and shape of the anisotropy, are extremely useful in identifying secondary structure content. Further, multinuclear correlations between these CSA parameters can clearly distinguish between various secondary structure elements such as helices and sheets. ©Adenine Press (2010).

KEYWORDS: amino acid, ab initio calculation; alpha helix; anisotropy; article; beta sheet; controlled study; correlation analysis; peptide mapping; priority journal; protein conformation; protein secondary structure; proton nuclear magnetic resonance, Anisotropy; Nitrogen Isotopes; Nuclear Magnetic Resonance, Biomolecular; Protein Structure, Secondary; Proteins

www.tandfonline.com/doi/abs/10.1080/07391102.2010.10507339

DOI:10.1080/07391102.2010.10507339

59. Sukhjeet Sidhu**., Jagdeep S .Deep.,** R C Sobti., V L Sharma., Hitender Thakur **(2010)** *Methylation pattern of MGMT gene in relation to age, smoking, drinking and dietary habits as epigenetic biomarker in prostate cancer patients.* **Genetic Engineering and Biotechnology Journal, GEBJ-8 1**

ABSTRACT: Epigenetic control of gene transcription is an important step for normal human development and cellular differentiation. Although alterations in DNA methylation pattern is a well-defined epigenetic change linked to human cancers and other diseases., inter-individual epigenetic variations in normal and cancer tissues due to ageing, smoking, drinking and meat-eating are poorly characterized. Population based studies are required to improve our understanding of epigenetic changes leading to progression of cancer. In this study, the methylation pattern of MGMT gene was studied in 100 tissue samples of prostate cancer patients along with 50 tissue samples of Benign Prostatic Hyperplasia cases and 100 blood samples from healthy individuals as controls. The results establish that the methylation pattern increases with age in BPH and healthy individuals whereas the maximum probability of developing prostate cancer is in the age group of 51-60 yrs. It is again proved in the study that smoking, drinking and non-vegetarian diet has a significant contribution in hypermethylation of MGMT gene, thus signifying that the methylation pattern can be designated as epigenetic biomarker in prostate cancer patients where the diagnosis is not well defined in the early stages of tumorigenesis.

KEYWORDS: biological marker; bisulfite; genomic DNA; methylated DNA protein cysteine methyltransferase, adult; age distribution; aged; article; cancer patient; carcinogenesis; controlled study; DNA methylation; DNA modification; drinking; eating habit; epigenetics; gene; gene expression; genetic risk; human; human tissue; major clinical study; mgmt gene; molecular genetics; prevalence; prostate cancer; prostate hypertrophy; smoking.

http://astonjournals.com/manuscripts/Vol2010/GEBJ-8_Vol2010.pdf

60. Anu Sabhlok . (2010) National identity in relief . **Geoforum, 41 (5), pp. 743- 751.**

ABSTRACT: This paper explores disaster relief as a medium, through which national identity manifests, circulates and is produced in local spaces. The objective is to move beyond studies of nationalism that emphasize solely the national scale (or the scale of the state) and to make visible the role of women as productive rather than merely reproductive subjects of national communities. The paper is based on over a year of ethnographic field work conducted between the years 2001-2005, in post-earthquake (2001) and in post-Godhra (2002) Gujarat, India. © 2010 Elsevier Ltd.

KEYWORDS: Disaster relief; Ethnography; Gender; Gujarat; India; Nationalism; Scale; SEWA; Women

KEYWORDS: disaster relief; fieldwork; gender issue; national identity; nationalism; womens status, Gujarat; India

http://www.sciencedirect.com/science/article/pii/S0016718510000485

http://dx.doi.org/10.1016/j.geoforum.2010.04.006

61. N.K.Singh, P., Tripathi, M.K.Bharty., A.K.Srivastava., **Sanjay Singh,** R.J.Butcher **(2010)** *Ni(II) and Mn(II) complexes of NNS tridentate ligand N′-[(2-methoxyphenyl)carbonothioyl]pyridine-2-carbohydrazide (H 2mcph): Synthesis, spectral and structural characterization.* **Polyhedron, 29 (8), pp. 1939-1945.**

ABSTRACT: The ligand N′-[(2-methoxyphenyl)carbonothioyl]pyridine-2-carbohydrazide (H_2mcph), having NNS donor sequence, has been found to form $[Ni(Hmcph)_2]\cdot CH_2Cl_2\cdot 0.5C_6H_6$ and $[Mn(Hmcph)_2]\cdot 2H_2O$ which have been characterized by spectroscopic and spectrometric techniques including magnetic susceptibility measurements and single crystal X-ray of both complexes. The compounds crystallize in the triclinic and monoclinic systems with the space group P over(1,¯) and P2(1)/c, respectively with a distorted octahedral geometry about the M(II) center. The ligand is coordinated through the ring nitrogen, hydrazinic N and thione sulfur. The hydrazinic nitrogen coordinates with a shorter M-N distance than the ring nitrogen and the bond lengths in the chelate ring systems are intermediate between single and double bond distances, suggesting considerable delocalization of charge. © 2010 Elsevier Ltd. All rights reserved.

KEYWORDS: Crystal structure; Ni(II) and Mn(II) complexes; Thiocarbohydrazide

http://www.sciencedirect.com/science/article/pii/S0277538710001361
http://dx.doi.org/10.1016/j.poly.2010.03.005

62. Indranil Biswas., Yogish Holla., **Chanchal Kumar (2010)** On moduli spaces of parabolic vector bundles of rank 2 over ℂℙ1 . **Michigan Mathematical Journal, 59 (2), pp. 467-479.**

http://projecteuclid.org/DPubS?service=UI&version=1.0&verb=Display&handle=euclid.mmj/1281531467

63. Pradeep Kumar., **N. Sathyamurthy (2010)** *Potential energy curves for neutral and multiply charged carbon monoxide*. **Pramana - Journal of Physics, 74 (1), pp. 49-55.**

ABSTRACT: Potential energy curves of various electronic states of CO^{n+} ($0 \geq n \geq 6$) are generated at MRCI/CASSCF level using cc-pvQZ basis set and the results are compared with available experimental and theoretical data. © Indian Academy of Sciences.

KEYWORDS: Ab initio calculations; Basis sets; Multi reference configuration interactions; Potential energy curves, Band structure; Carbon monoxide; Electronic states; Excited states; Ground state; Sulfur compounds, Potential energy

http://link.springer.com/article/10.1007%2Fs12043-010-0006-y?LI=true#page-1

PACS Nos 31.15.Ar; 31.25.Nj; 31.25.Jf; 31.25.Eb

64. Sukhdeep Kumar., Kusum Lata., Srirupa Mukhopadhyay., Tapan K. Mukherjee (2010) *Role of estrogen receptors in pro-oxidative and anti-oxidative actions of estrogens: A perspective* . **Biochimica et Biophysica Acta - General Subjects, 1800 (10), pp. 1127-1135.**

ABSTRACT: Background: Estrogens are steroid hormones responsible for the primary and secondary sexual characteristics in females. While pre-menopausal women use estrogens as the main constituents of contraceptive pills, post-

menopausal women use the same for Hormone Replacement Therapy. Estrogens produce reactive oxygen species by increasing mitochondrial activity and redox cycling of estrogen metabolites. The phenolic hydroxyl group present at the C3 position of the A ring of estrogens can get oxidized either by accepting an electron or by losing a proton. Thus, estrogens might act as pro-oxidant in some settings, resulting in complicated non-communicable diseases, namely, cancer and cardiovascular disorders. However, in some other settings the phenolic hydroxyl group of estrogens may be responsible for the anti-oxidative beneficial functions and thus protect against cardiovascular and neurodegenerative diseases. Scope of review: To date, no single review article has mentioned the implication of estrogen receptors in both the pro-oxidative and anti-oxidative actions of estrogens. Major conclusion: The controversial role of estrogens as pro-oxidant or anti-oxidant is largely dependent on cell types, ratio of different types of estrogen receptors present in a particular cell and context specificity of the estrogen hormone responses. Both pro-oxidant and anti-oxidant effects of estrogens might involve different estrogen receptors that can have either genomic or non-genomic action to manifest further hormonal response. General significance: This review highlights the role of estrogen receptors in the pro-oxidative and anti-oxidative actions of estrogens with special emphasis on neuronal cells. © 2010 Elsevier B.V.

KEYWORDS: 17 epiestriol; 2 hydroxyestradiol; 2,3 estradiolquinone; 3,4 estradiolquinone; 4 hydroxyestradiol; 4 hydroxyestrone; catechol estrogen; estradiol; estradiol derivative; estriol; estrogen; estrogen derivative; estrogen receptor alpha; estrogen receptor beta; estrone; ethinylestradiol; fulvestrant; genistein; n butyl 11 (3,17beta dihydroxyestra 1,3,5(10) trien 7alpha yl) n methylundecanamide; nitric oxide; phenol; phytoestrogen; progesterone; quinone derivative; raloxifene; reactive oxygen metabolite; steroid hormone; tamoxifen; thioredoxin; unclassified drug; unindexed drug, Alzheimer disease; antioxidant activity; breast cancer; cardiovascular disease; cell type; cerebrovascular accident; degenerative disease; drug dose increase; drug mechanism; drug receptor binding; drug structure; drug withdrawal; estrogen metabolism; heart protection; hormone action; hormone response; hormone substitution; human; ischemic heart disease; lung embolism; menopausal syndrome; mitochondrial energy transfer; mitochondrial respiration; multiinfarct dementia; nerve cell; neuroprotection; nonhuman; oral contraception; oxidation reduction reaction; postmenopause osteoporosis; priority journal; protein expression; protein

localization; review; structure activity relation, Animals; Antioxidants; Cardiovascular Diseases; Contraceptives, Oral, Hormonal; Estrogen Replacement Therapy; Estrogens; Female; Humans; Male; Mitochondria; Neoplasms; Neurodegenerative Diseases; Neurons; Organ Specificity; Oxidants; Oxidation-Reduction; Premenopause; Receptors, Estrogen

http://www.sciencedirect.com/science/article/pii/S0304416510001182

http://dx.doi.org/10.1016/j.bbagen.2010.04.011

65. Ravi Chand Singh., Onkar Singh, Manmeet Pal Singh., **Paramdeep Singh Chandi.,** R. Thangaraj **(2010)** *Sensing behaviour of nanosized zinc-tin composite oxide towards liquefied petroleum gas and ethanol*. **Materials Research Bulletin, 45 (9), pp. 1162-1164.**

ABSTRACT: A chemical route has been used to synthesize composite oxides of zinc and tin. An ammonia solution was added to equal amounts of zinc and tin chloride solutions of same molarities to obtain precipitates. Three portions of these precipitates were annealed at 400, 600 and 800 °C, respectively. Results of X-ray diffraction and transmission electron microscopy clearly depicted coexistence of phases of nano-sized SnO^2, ZnO, Zn^2SnO^4 and $ZnSnO^3$. The effect of annealing on structure, morphology and sensing has been observed as well. It has been observed that annealing promoted growth of Zn $2SnO^4$ and $ZnSnO^3$ at the expense of zinc. The sensing response of fabricated sensors from these materials to 250 ppm LPG and ethanol has been investigated. The sensor fabricated from powder annealed at 400 °C responded better to LPG than ethanol. © 2010 Elsevier Ltd. All rights reserved.

KEYWORDS: A. Composites; A. Oxides; Ammonia solution; Chemical routes; Chemical synthesis; Coexistence of phasis; Composite oxide; Fabricated sensors; Nano-sized; Sensing response; Tin chlorides; ZnO, Annealing; Butane; Chlorine compounds; Complexation; Ethanol; Gas industry; Liquefied petroleum gas; Nanostructures; Scanning electron microscopy; Sensors; Synthesis (chemical); Tin; Tin oxides; Titanium compounds; Transmission electron microscopy; X ray diffraction; Zinc oxide, Zinc

http://www.sciencedirect.com/science/article/pii/S0025540810001923

http://dx.doi.org/10.1016/j.materresbull.2010.05.025,

66. Brijesh Kumar Mishra., J. Samuel Arey ., **N. Sathyamurthy (2010)** *Stacking and spreading interaction in N-heteroaromatic systems* . **Journal of Physical Chemistry A, 114 (36), pp. 9606-9616.**

ABSTRACT: π-π interactions in heteroaromatic systems are ubiquitous in biological systems. In the present study, stabilization energies of stacked and hydrogen-bonded dimers of N-heteroaromatic systems (pyridine, pyrazine, sym-triazine, and sym-tetrazine) have been computed using a benchmark quality coupled cluster through the perturbative triples (CCSD(T)) method at the estimated complete basis set (CBS) limit. In the case of stacking, monomer units are found to be stacked in parallel planes with displaced geometries. The stabilization energies for the most stable stacked geometry of pyridine, pyrazine, sym-triazine, and sym-tetrazine dimers are found to be -3.39, -4.14, -4.02, and -3.90 kcal/mol, respectively at the est. CCSD(T)/CBS level of theory, which is clearly larger than the stabilization energy for the most stable geometry of the benzene dimer. In the case of spreading, hydrogen bonded dimers and trimers are stabilized by weak C-H · · · N interactions. The stabilization energies for the stacked and the spread out complexes are found to be comparable. The stabilization energy for the trimers is computed using the MP2, MP3, and B3LYP-D methods. The present study is aimed at unraveling the basis of preferred conformations of N-heteroaromatic dimers. These model systems explain partly the stability of double helical DNA and RNA structures that are formed by stacking and hydrogen bonding between nucleic acid bases. © 2010 American Chemical Society.

KEYWORDS: Benzene dimers; CCSD; Complete basis set limit; Coupled clusters; Double-helical; Heteroaromatic systems; Hydrogen bondings; Hydrogen-bonded dimers; Model system; Monomer units; Nucleic acid basis; Parallel planes; Pyrazines; RNA structures; Spreading interaction; Stabilization energy; Tetrazines, Benchmarking; Benzene; Complexation; Dimers; Electric circuit breakers; Geometry; Hydrogen; Hydrogen bonds; Nucleic acids; Pyridine; RNA, Stabilization, DNA; heterocyclic compound; nitrogen; RNA, article; chemical structure; chemistry; conformation; dimerization; hydrogen bond; thermodynamics, Dimerization; DNA; Heterocyclic Compounds; Hydrogen Bonding; Models, Molecular; Molecular Conformation; Nitrogen; RNA; Thermodynamics .

http://pubs.acs.org/doi/abs/10.1021/jp908941u

DOI: 10.1021/jp908941u

67. A. Kenfack ., **Kamal P. Singh (2010)** *Stochastic Resonance in coupled Underdamped Bistable Systems,* **Phys Rev E 82, 046224.**

ABSTRACT : We study onset and control of stochastic resonance (SR) phenomenon in two driven bistable systems, mutually coupled and subjected to independent noises, taking into account the influence of both the inertia and the coupling. In the absence of coupling, we found two critical damping parameters: one for the onset of SR and another for which SR is optimum. We then show that in weakly coupled systems, emergence of SR is governed by chaos. A strong coupling between the two oscillators induces coherence in the system; however, the systems do not synchronize no matter what the coupling is. Moreover, a specific coupling parameter is found for which the SR of each subsystem is optimum. Finally, a scheme for controlling SR in such coupled systems is proposed by introducing a phase difference between the two coherent driving forces.

http://pre.aps.org/abstract/PRE/v82/i4/e046224

DOI:10.1103/PhysRevE.82.046224

68. Pratibha Kapoor., Ajay Pal Singh Pannu., Mukesh Sharma., Maninder Singh Hundal., **Ramesh Kapoor (2010)** *Syntheses and X-ray crystal structures of five- and six-coordinate copper(II) complexes of N,N,N′,N′-tetraalkylpyridine-2,6-dicarboxamides containing-OClO$_3$ and-OSO$_2$CF$_3$ counter ions.* **Journal of Coordination Chemistry, 63 (20), pp. 3635-3647.**

ABSTRACT: Reactions of anhydrous copper(II) chloride with NaX (1 : 1 or 1 : 2) and AgX (1 : 2) containing appropriate N,N,N',N'-tetraalkylpyridine-2,6-dicarboxamides(O-daap) in CH_3CN yield monosubstituted five-coordinate $[Cu(L_1)C\ l(CF_3SO_3)]$ (1), $[Cu(L_2)Cl(ClO_4)]$ (2), $[Cu(L_3)Cl(ClO_4)]$ (3), and six-coordinate $[Cu(L_2)(CF_3SO_3)_2]\ H_2O$ (4) (X = -$OClO_3$ and-OSO_2CF_3; L_1 = N,N,N',N'-tetraethylpyridine-2,6- dicarboxamides; L_2 = N,N,N',N'-tetraisopropylpyridine-2,6-dicarboxamides; L_3 = N,N,N',N'-tetraisobutylpyridine-2,6-dicarboxamides). The structures of these complexes have been determined by X-ray crystallography. The Cu^{2+} in 1-3 adopts distorted square-pyramidal geometry, while 4 exhibits octahedral structure. Steric factors in conjunction with lattice effects and the nature of the anions are responsible for the variety in coordination spheres. These compounds undergo extensive intermolecular H-bonding to give to 2-D sheets extending along various planes. © 2010 Taylor & Francis.

KEYWORDS: Alkyl-substituted pyridine-2,6-dicarboxamides; Metathetical reactions; Steric and anionic effects; X-ray crystal structures

http://www.tandfonline.com/doi/abs/10.1080/00958972.2010.517267

DOI:10.1080/00958972.2010.517267

69. Pratibha Kapoor., Ajay Pal Singh Pannu., Mukesh Sharma., Maninder Singh Hundal., **Ramesh Kapoor.**, Montserrat Corbella., Núria Aliaga-Alcalde **(2010)** *Syntheses, X-ray crystal structure and magnetic studies of a new dinuclear Cu* ^{II} *complex,* $[Cu_2(\mu\text{-}Cl)_2L_2Cl_2]\cdot 2CH_3CN$*, L: N,N,N′,N′-tetraisopropylpyridine-2,6-dicarboxamide* **Journal of Molecular Structure, 981 (1-3), pp. 40-45.**

ABSTRACT: Reaction of anhydrous copper(II) chloride with N,N,N′,N′-tetraisopropylpyridine-2,6-dicarboxamide (L) leads to the synthesis of $[Cu_2Cl_4L_2]\cdot 2CH_3CN$, 1. The ligand coordinates to each Cu^{II} ion in a bidentate fashion through pyridine nitrogen and only one of the carbonyl oxygen atoms of the amide group rather than using tridentate coordination mode O-N-O. The structure can be described as a dichloro bridged centrosymmetric dimer where the two copper centers are pentacoordinated in a square pyramidal fashion. The two pyramids are arranged sharing a basal edge with their apical positions oriented opposite to each other. The crystal packing investigations show a 2D sheet in the lattice held together by dimeric acetonitrile entities. Complex 1 shows weak antiferromagnetic coupled Cu^{2+} ions. © 2009 Elsevier B.V. All rights reserved.

KEYWORDS: Amide groups; Antiferromagnetics; Apical positions; Basal edges; Carbonyl oxygen atoms; Centrosymmetric dimers; Complex 1; Coordination modes; Copper centers; Copper chlorides; Crystal packings; Dinuclear; Ligand coordinates; Magnetic studies; Pentacoordinated; Pyridine nitrogen; X ray crystal structures, Acetonitrile; Amides; Antiferromagnetic materials; Antiferromagnetism; Chlorine compounds; Oxygen; Synthesis (chemical); X rays, Crystal structure http://www.sciencedirect.com/science/article/pii/S0022286010005892

http://dx.doi.org/10.1016/j.molstruc.2010.07.021

70. Ashok Ajoy., **Pranaw Rungta (2010)** *Svetlichny's inequality and genuine tripartite nonlocality in three-qubit pure states*, **Phys. Rev. A 81, 052334**

ABSTRACT: The violation of the Svetlichny's inequality (SI) [Phys. Rev. D **35** 3066 (1987)] is sufficient but not necessary for genuine tripartite nonlocal correlations. Here we quantify the relationship between tripartite entanglement and the maximum expectation value of the Svetlichny operator (which is bounded from above by the inequality) for the two inequivalent subclasses of pure three-qubit states: the Greenberger-Horne-Zeilinger (GHZ) class and the W class. We show that the maximum for the GHZ-class states reduces to Mermin's inequality [Phys. Rev. Lett. **65** 1838 (1990)] modulo a constant factor, and although it is a function of the three tangle and the residual concurrence, large numbers of states do not violate the inequality. We further show that by design SI is more suitable as a measure of genuine tripartite nonlocality between the three qubits in the W-class states, and the maximum is a certain function of the bipartite entanglement (the concurrence) of the three reduced states, and only when their sum attains a certain threshold value do they violate the inequality.

http://pra.aps.org/abstract/PRA/v81/i5/e052334

DOI:10.1103/PhysRevA.81.052334

71. Manish Dev Shrimali., Swarup Poria.., **Sudeshna Sinha (2010)** *Under what kind of parametric fluctuations is spatiotemporal regularity the most robust?* **Pramana - Journal of Physics, 74 (6), pp. 895-906.**

ABSTRACT: It was observed that the spatiotemporal chaos in lattices of coupled chaotic maps was suppressed to a spatiotemporal fixed point when some fractions of the regular coupling connections were replaced by random links. Here we investigate the effects of different kinds of parametric fluctuations on the robustness of this spatiotemporal fixed point regime. In particular we study the spatiotemporal dynamics of the network with noisy interaction parameters, namely fluctuating fraction of random links and fluctuating coupling strengths. We consider three types of fluctuations: (i) noisy in time, but homogeneous in space; (ii) noisy in space, but fixed in time; (iii) noisy in both space and time. We find that the effect of different kinds of parametric noise on the dynamics is quite distinct: quenched spatial fluctuations are the most detrimental to spatiotemporal regularity; spatiotemporal fluctuations yield phenomena similar to that observed when parameters are held constant at the mean value, and interestingly, spatiotemporal regularity is most robust under spatially uniform temporal fluctuations, which in fact yields a larger fixed point range than that obtained under constant mean-value parameters. © Indian Academy of Sciences.

KEYWORDS: Chaotic map; Coupled map lattices; Coupling strengths; Fixed points; Interaction parameters; Mean values; Networks; Random links; Space and time; Spatial fluctuation; Spatio-temporal dynamics; Spatio-temporal fluctuations; Spatiotemporal chaos; Temporal fluctuation; Yield phenomenon, Crystal lattices; Dynamics, Chaotic systems

http://arxiv.org/pdf/0807.0842v1.pdf

http://link.springer.com/article/10.1007%2Fs12043-010-0082-z?LI=true#page-1

72. Ramandeep S. Johal (2010) *Universal efficiency at optimal work with Bayesian statistics.* **Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 82 (6), art. no. 061113, .**

ABSTRACT: If the work per cycle of a quantum heat engine is averaged over an appropriate prior distribution for an external parameter a, the work becomes optimal at Curzon-Ahlborn (CA) efficiency. More general priors of the form Π (a) $\propto 1/ a\gamma$ yield optimal work at an efficiency which stays close to CA value, in particular near equilibrium the efficiency scales as one-half of the Carnot value. This feature is analogous to the one recently observed in literature for certain models of finite-time thermodynamics. Further, the use of Bayes' theorem implies that the work estimated with posterior probabilities also bears close analogy with the classical formula. These findings suggest that the notion of prior information can be used to reveal thermodynamic features in quantum systems, thus pointing to a connection between thermodynamic behavior and the concept of information. © 2010 The American Physical Society.

KEYWORDS: Bayes' theorem; Bayesian statistics; Finite time thermodynamics; Posterior probability; Prior distribution; Prior information; Quantum heat engines; Quantum system; Thermodynamic behaviors; Work per cycle, Quantum electronics; Quantum optics; Thermodynamics, Optimization

http://arxiv.org/abs/1002.4941

http://pre.aps.org/abstract/PRE/v82/i6/e061113

DOI: 10.1103/PhysRevE.82.061113

73. S.Begam Elavarasi., **Amrita Kumari., Kavita Dorai (2010)** *Using the chemical shift anisotropy tensor of carbonyl backbone nuclei as a probe of secondary structure in proteins.* **Journal of Physical Chemistry A, 114 (18), pp. 5830-5837.**

ABSTRACT: This study seeks to establish that the chemical shift anisotropy (CSA) tensor of the backbone carbonyl (^{13}C) nucleus is a useful indicator of secondary structure elements in proteins. The CSA tensors of protein backbone nuclei in different secondary structures were computed for experimentally determined dihedral angles using ab initio methods and by calculating the CSA tensor for a model peptide over the entire dihedral angle space. It is shown that 2D and 3D cluster plots of CSA tensor parameters for ^{13}C' nuclei are able to distinguish between different secondary structure elements with little to no overlap. As evidenced by multinuclear 2D plots, the CSA of the ^{13}C nucleus when correlated with different CSA parameters of the other backbone nuclei (such as C^{α} or $1^{H\alpha}$) is also useful in secondary structure identification. The differentiation of α-helix versus β-sheet motifs (the most populated regions of the Ramachandran map) for experimentally determined values of the carbonyl CSA tensor for proteins ubiquitin and binase (obtained from the literature) agrees well with the quantum chemical predictions. © 2010 American Chemical Society.

KEYWORDS: 3D clusters; [carbonyl; Ab initio method; Backbone carbonyl; Chemical shift anisotropy; Dihedral angles; Model peptides; Protein backbone; Quantum chemical; Secondary structure elements; Secondary structures; Ubiquitin, Anisotropy; Carbonylation; Proteins; Tensors, Chemical shift, carbon; protein, anisotropy; article; biological model; chemistry; protein secondary structure; quantum theory, Anisotropy; Carbon; Models, Biological; Protein Structure, Secondary; Proteins; Quantum Theory

http://pubs.acs.org/doi/abs/10.1021/jp9113199

DOI:10.1021/jp9113199

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74. Soma Duley., Santanab Giri., **Narayanasami Sathyamurthy**, Rafael Islas, Gabriel Merino, Pratim Kumar Chattaraj (**2011**) A*romaticity and hydrogen storage capability of planar* $N_6{}^{4-}$*and* $N_4{}^{2}$ *rings.* **Chemical Physics Letters, 506 (4-6), pp. 315-320.**

ABSTRACT: Theoretical investigation on planar N_6^{4-} and N_4^{2-} rings has been performed. The aromaticity of the rings has been analyzed through their nucleus independent chemical shift (NICS) values as well as the σ- and π-contribution of the Z-component of the induced magnetic field. Counter to a previously reported result [Chem. Phys. Lett. 432 (2006) 331], the $N_6{}^{4-}$ ring is found to be a local minimum and aromatic with planar D_{6h} symmetry. The $N_6{}^{2-}$ ring exhibits conflicting aromaticity like AlN_4^{4-}. Both the N_6^{4-} and N_4^{2-} rings can be stabilized in presence of suitable counter cations and systems like N_6Ca_2 and N_4Li_2 can trap molecular hydrogen. © 2011 Elsevier B.V. All rights reserved.

KEYWORDS: AlN; Aromaticities; Counter cations; Induced magnetic fields; Local minimums; Molecular hydrogen; Nucleus independent chemical shifts; Storage capability; Theoretical investigations, Aromatization; Chemical analysis; Hydrogen; Magnetic fields, Hydrogen storage

http://ac.els-cdn.com/S000926141100306X/1-s2.0-S000926141100306X-main.pdf?_tid=e52201c2-8df9-11e2-9fac-00000aacb35f&acdnat=1363411700_53a9f17d76e9b52312741b705b95cea9
http://dx.doi.org/10.1016/j.cplett.2011.03.037

75. Ajay Pal Singh Pannu., Pratibha Kapoor., Geeta Hundal., **Ramesh Kapoor.,** Martin Martinez-Ripoll., Maninder Singh Hundal (**2011**) *A self assembled 3-D network propagated by coordination polymerization and H-bonding: Synthesis and X-ray crystal structure of* $[\{Co(L)_2(H_2O)_2\}(ClO_4)_2(CH_3COCH_3)_2(H_2O)_2]_n$*, where L = N,N- diisopropylisonicotinamide* . **Journal of Coordination Chemistry, 64 (9), pp. 1566-1577**.

ABSTRACT: Reaction of $Co(ClO_4)_{2..}6H_2O$ with N,N-diisopropylisonicotinamide (L) has yielded a 1-D coordination polymer $[\{Co(L)_2(H_2O)_2\}(ClO_4)_2(CH_3COCH_3)_2(H_2O)_2]n(1)$. Complex 1 has been characterized by infrared (IR) and UV-Vis spectroscopies, thermal analysis, and single crystal X-ray diffraction techniques. The structure has alternate arrangement of parallel 1-D cationic metal-ligand chains and H-bonded anionic chains containing perchlorate, acetone and water in the lattice. Further hydrogen bonding among both chains leads to formation of 2-D networks along almost perpendicular planes. Interpenetrations of such perpendicular 2-D sheets create a 3-D supramolecular structure. © 2011 Taylor & Francis.

KEYWORDS: Coordination network; Crystal structure; H-Bonding; N,N-Diisopropylisonicotinamide; Thermal stability

http://www.tandfonline.com/doi/full/10.1080/00958972.2011.574286

DOI:10.1080/00958972.2011.574286

76. Mukherjee, Tapan K., Paul, Karan., Mukhopadhyay, Srirupa. (2011) *Cell signaling molecules as drug targets in lung cancer: An overview*. **Current Opinion in Pulmonary Medicine, 17 (4), pp. 286-291.**

ABSTRACT: Lung being one of the vital and essential organs in the body, lung cancer is a major cause of mortality in the modern human society. Lung cancer can be broadly subdivided into nonsmall cell lung cancer (NSCLC) and small cell lung cancer (SCLC). Although NSCLC is sometimes treated with surgery, the advanced and metastatic NSCLC and SCLC usually respond better to chemotherapy and radiation. The most important targets of these chemotherapeutic agents are various intracellular signaling molecules. The primary focus of this review article is to summarize the description of various cell signaling molecules involved in lung cancer development and their regulation by chemotherapeutic agents. RECENT FINDINGS: Extensive research work in recent years has identified several cellular signaling molecules that may be intricately involved in the complexity of lung cancer. Some of these cell signaling molecules are epidermal growth factor receptors, vascular endothelial growth factor receptors, mammalian target of rapamycin, mitogen-activated protein kinase phosphatase-1, peroxisome proliferator-activated

receptor-gamma, matrix metalloproteinases and receptor for advanced glycation end-products. SUMMARY: The present review will strengthen our current knowledge regarding the efficacy of the above-mentioned cell signaling molecules as potential beneficial drug targets against lung cancer. © 2011 Lippincott Williams & Wilkins, Inc.

KEYWORDS: acetylsalicylic acid; antineoplastic agent; batimastat; bevacizumab; cetuximab; cisplatin; epidermal growth factor receptor; epidermal growth factor receptor kinase; erlotinib; gefitinib; gelatinase A; gelatinase B; immunoglobulin enhancer binding protein; matrix metalloproteinase; mitogen activated protein kinase 1; peroxisome proliferator activated receptor; peroxisome proliferator activated receptor gamma; prinomastat; protein p53; protein serine threonine kinase; protein tyrosine kinase; rosiglitazone; selective estrogen receptor modulator; somatomedin receptor; tissue inhibitor of metalloproteinase 1; transcription factor Slug; troglitazone; vasculotropin; vasculotropin inhibitor, apoptosis; article; cancer chemotherapy; cancer growth; carcinogenesis; cigarette smoking; distant metastasis; DNA damage; drug efficacy; drug targeting; enzyme activity; extracellular matrix; gene; gene mutation; human; immunocytochemistry; intracellular signaling; lung cancer; lung non small cell cancer; lung small cell cancer; nonhuman; phase 1 clinical trial (topic); phase 2 clinical trial; prognosis; protein expression; systemic disease, Carcinoma, Non-Small-Cell Lung; Carcinoma, Small Cell; Humans; Lung Neoplasms; Molecular Targeted Therapy; Signal Transduction

http://journals.lww.com/co-pulmonarymedicine/Abstract/2011/07000/Cell_signaling_molecules_as_drug_targets_in_lung.14.aspx

doi: 10.1097/MCP.0b013e328347bda6

77. Amit Kumar Yadav., **Anand Kumar Bachhawat (2011)** *CgCYN1, a plasma membrane cystine-specific transporter of Candida glabrata with orthologues prevalent among pathogenic yeast and fungi.* **Journal of Biological Chemistry, 286 (22), pp. 19714-19723.**

ABSTRACT: We describe a novel plasma membrane cystine transporter, CgCYN1, from Candida glabrata, the first such transporter to be described from yeast and fungi. C. glabrata met15Δ strains, organic sulfur auxotrophs, were observed to utilize cystine as a sulfur source, and this phenotype was exploited in the discovery of CgCYN1. Heterologous expression of CgCYN1 in Saccharomyces cerevisiae met15Δ strains conferred the ability of S. cerevisiae strains to grow on cystine. Deletion of the CgCYN1 ORF (CAGL0M00154g) in C. glabrata met15Δ strains caused abrogation of growth on cystine with growth being restored when CgCYN1 was reintroduced. The CgCYN1 protein belongs to the amino acid permease family of transporters, with no similarity to known plasma membrane cystine transporters of bacteria and humans, or lysosomal cystine transporters of humans/yeast. Kinetic studies revealed a K m of 18 ± 5 μM for cystine. Cystine uptake was inhibited by cystine, but not by other amino acids, including cysteine. The structurally similar cystathionine, lanthionine, and selenocystine alone inhibited transport, confirming that the transporter was specific for cystine. CgCYN1 localized to the plasma membrane and transport was energy-dependent. Functional orthologues could be demonstrated from other pathogenic yeast like Candida albicans and Histoplasma capsulatum, but were absent in Schizosaccharomyces pombe and S. cerevisiae. © 2011 by The American Society for Biochemistry and Molecular Biology, Inc.

KEYWORDS: Candida albicans; Candida glabrata; Energy dependent; Heterologous expression; Kinetic study; Lanthionines; Organic sulfur; Orthologues; Pathogenic yeast; Plasma membranes; S.cerevisiae; Saccharomyces cerevisiae; Schizosaccharomyces pombe; Selenocystine; Sulfur source, Amino acids; Candida; Cell membranes; Plasmas; Selenium compounds; Sulfur, Yeast, cystathionine; cysteine; cystine; lanthionine; selenocystine, amino acid transport; article; Candida albicans; Candida glabrata; cell membrane; cellular distribution; controlled study; CYN1 gene; fungal gene; fungal strain; fungus growth; gene deletion; heterologous expression; Histoplasma capsulatum; nonhuman; open reading frame; orthology; priority journal; protein localization; Saccharomyces cerevisiae; Schizosaccharomyces pombe, Amino Acid Transport Systems, Neutral; Biological Transport; Candida glabrata; Cysteine; Fungal Proteins; Histoplasma; Saccharomyces cerevisiae; Schizosaccharomyces; Species Specificity, Ajellomyces capsulatus; Candida albicans; Candida glabrata; Fungi; Saccharomyces cerevisiae; Schizosaccharomyces pombe

http://www.jbc.org/content/286/22/19714.short

DOI:10.1074/jbc.M111.240648

78. Neha Jain., Mily Bhattacharya., Samrat Mukhopadhyay (2011) *Chain collapse of an amyloidogenic intrinsically disordered protein*. **Biophysical Journal, 101 (7), pp. 1720-1729.**

ABSTRACT: Natively unfolded or intrinsically disordered proteins (IDPs) are under intense scrutiny due to their involvement in both normal biological functions and abnormal protein misfolding disorders. Polypeptide chain collapse of amyloidogenic IDPs is believed to play a key role in protein misfolding, oligomerization, and aggregation leading to amyloid fibril formation, which is implicated in a number of human diseases. In this work, we used bovine κ-casein, which serves as an archetypal model protein for amyloidogenic IDPs. Using a variety of biophysical tools involving both prediction and spectroscopic techniques, we first established that monomeric κ-casein adopts a collapsed premolten-globule-like conformational ensemble under physiological conditions. Our time-resolved fluorescence and light-scattering data indicate a change in the mean hydrodynamic radius from ~4.6 nm to ~1.9 nm upon chain collapse. We then took the advantage of two cysteines separated by 77 amino-acid residues and covalently labeled them using thiol-reactive pyrene maleimide. This dual-labeled protein demonstrated a strong excimer formation upon renaturation from urea- and acid-denatured states under both equilibrium and kinetic conditions, providing compelling evidence of polypeptide chain collapse under physiological conditions. The implication of the IDP chain collapse in protein aggregation and amyloid formation is also discussed. © 2011 Biophysical Society.

KEYWORDS: amyloid protein; casein; peptide; pyrene; pyrene derivative, amino acid sequence; animal; article; biology; cattle; chemistry; fluorescence polarization; fluorescence resonance energy transfer; kinetics; light; metabolism; molecular genetics; protein multimerization; radiation scattering, Amino Acid Sequence; Amyloidogenic Proteins; Animals; Caseins; Cattle; Computational Biology; Fluorescence Polarization; Fluorescence Resonance Energy Transfer; Kinetics; Light; Molecular Sequence Data; Peptides; Protein Multimerization; Pyrenes; Scattering, Radiation, Bovinae

http://www.cell.com/biophysj/abstract/S0006-3495%2811%2900970-2

doi:10.1016/j.bpj.2011.08.024

79. Wensheng Cao., **Krishnendu Gongopadhyay (2011)** *Commuting isometries of the complex hyperbolic space* . **Proceedings of the American Mathematical Society, 139 (9), pp. 3317-3326**.

ABSTRACT: Let Hnℂ denote the complex hyperbolic space of dimension n. The group U(n, 1) acts as the group of isometries of Hnℂ. In this paper we investigate when two isometries of the complex hyperbolic space commute. Along the way we determine the centralizers. © 2011 American Mathematical Society.

KEYWORDS: Centralizers; Complex hyperbolic space; Isometries

arxiv.org/pdf/1002.2479

80. Krishnendu Gongopadhyay (2011) *Conjugacy Classes in Möbius groups .* **Geometriae Dedicata, 151 (1), pp. 245-258.**

ABSTRACT: Let ℍn+1 denote the n + 1-dimensional (real) hyperbolic space. Let Sn denote the conformal boundary of the hyperbolic space. The group of conformal diffeomorphisms of Sn is denoted by M(n). Let Mo(n) be its identity component which consists of all orientation-preserving elements in M(n). The conjugacy classification of isometries in Mo(n) depends on the conjugacy of T and T-1 in Mo(n). For an element T in M(n), T and T-1 are conjugate in M(n), but they may not be conjugate in Mo(n). In the literature, T is called real if T is conjugate in Mo(n) to T-1. In this paper we classify real elements in Mo(n). Let T be an element in Mo(n). Corresponding to T there is an associated element To in SO(n+1). If the complex conjugate eigenvalues of To are given by {eiθj, e-iθj}, 0 < θj ≤ π, j = 1,. . ., k, then {θ1, . . ., θk} are called the rotation angles of T. If the rotation angles of T are distinct from each-other, then T is called a regular element. After classifying the real elements in Mo(n) we have parametrized the conjugacy classes of regular elements in Mo(n). In the parametrization, when T is not conjugate to T-1, we have enlarged the group and have considered the conjugacy class of T in M(n). We prove that each such conjugacy class can be induced with a fibration structure. © 2010 Springer Science+Business Media B.V.

KEYWORDS: Conjugacy classes; Hyperbolic space; Möbius groups; Real elements

http://link.springer.com/article/10.1007%2Fs10711-010-9531-6?LI=true#page-1

DOI: 10.1007/s10711-010-9531-6

81. Ajay Pal Singh Pannu., Pratibha Kapoor., Geeta Hundal., **Ramesh Kapoor.**, Martin Martinez-Ripoll., Rayond J. Butcher., Maninder Singh Hundal **(2011)** *Coordination driven or/and H-bonded Cu(II)-N,N-dialkylisonicotinamide frameworks*. **Polyhedron, 30 (10), pp. 1691-1702.**

ABSTRACT: Reactions of N,N-diisopropylisonicotinamide (L) with anhydrous $CuCl_2$, $CuBr_2$ and $Cu(ClO_4)_2\cdot$ $6H_2O$ yielded: (a) an ionic product with the molecular composition of $[CuL_2(H_2O)_4]\cdot 2[CuLCl_3]$ 1; (b) a coordination polymer $[CuL_2Br_2]n^2$ and (c) a mononuclear complex $[CuL_4(C_3H_8O)_2]\cdot(ClO_4)_2]3$, respectively. Similarly, the reaction of N,N-diisobutylisonicotinamide (L′) with $Cu(NO_3)_2\cdot 3H_2O$ yielded a coordination polymer $[\{CuL'_2(H_2O)_2\}(NO_3)_{2]\,n}$ 4. The ligands L and L′ coordinate in a monodentate fashion through the pyridine nitrogen atom to the metal centers in complexes 1 and 3. However, complexes 2 and 4 are coordination polymers in which the corresponding ligands (L and L′) act as bridging bidentate between metal centers to form 1D double chains. All the four complexes form networks through coordination polymerization and/or hydrogen bonding. © 2011 Elsevier Ltd. All rights reserved.

KEYWORDS: Coordination polymers; Hydrogen bonding; N,N-dialkylisonicotinamides; Thermal analysis; Trinuclear entity; X-ray structures

http://www.sciencedirect.com/science/article/pii/S0277538711002312

http://dx.doi.org/10.1016/j.poly.2011.03.047,

82. Mohan., **Visakhi.P.,** S.Ravi **(2011)** _Coral Reef Research in India: a Bibliometric Analysis (Part.1)_ ***Indian Journal of Agricultural Library and Information Services, Vol.*** **27 (1) Jan-June : 48 - 60p**

ABSTRACT : The part- I of this paper attempts to evaluate the coral reef research in India using Bibliometric tools for the period 1900 - 2000. The data has been extracted from ***"Bibliography on Indian coral reefs".*** It highlights research productivity by subjects, domains, institutions (Research and Academic) etc. The study examines authorship pattern, productivity on individual scientists and also identified the various countries participation. It analyzes the forms of communication, journals productivity and identified criteria for selection of the core journals for library. Suggested to create a database on coral reefs and to develop marine science at national level that would facilitate easy use of all categories of people.

KEYWORDS : Coral Reefs, Bibliometrics

83. George Thomas., Ramandeep S. Johal (2011) _Coupled quantum Otto cycle._ **Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 83 (3), art. no. 031135, .**

ABSTRACT: We study the one-dimensional isotropic Heisenberg model of two spin-1/2 systems as a quantum heat engine. The engine undergoes a four-step Otto cycle where the two adiabatic branches involve changing the external magnetic field at a fixed value of the coupling constant. We find conditions for the engine efficiency to be higher than in the uncoupled model; in particular, we find an upper bound which is tighter than the Carnot bound. A domain of parameter values is pointed out which was not feasible in the interaction-free model. Locally, each spin seems to cause a flow of heat in a direction opposite to the global temperature gradient. This feature is explained by an analysis of the local effective temperature of the spins. © 2011 American Physical Society.

KEYWORDS: Coupling constants; Effective temperature; Engine efficiency; External magnetic field; Global temperatures; Isotropic Heisenberg; Parameter values; Quantum heat engines; Uncoupled models; Upper Bound, Magnetic fields, Otto cycle

http://pre.aps.org/abstract/PRE/v83/i3/e031135

DOI: 10.1103/PhysRevE.83.031135

84. K.Srinivasan., I.Raja Mohamed., K.Murali., M.Lakshmanan., **Sudeshna Sinha** **(2011)** *Design of time delayed chaotic circuit with threshold controller* .**International Journal of Bifurcation and Chaos, 21 (3), pp. 725-735.**

ABSTRACT: A novel time delayed chaotic oscillator exhibiting mono- and double scroll complex chaotic attractors is designed. This circuit consists of only a few operational amplifiers and diodes and employs a threshold controller for flexibility. It efficiently implements a piecewise linear function. The control of piecewise linear function facilitates controlling the shape of the attractors. This is demonstrated by constructing the phase portraits of the attractors through numerical simulations and hardware experiments. Based on these studies, we find that this circuit can produce multi-scroll chaotic attractors by just introducing more number of threshold values. © 2011 World Scientific Publishing Company.

KEYWORDS: chaos; Chaotic attractors; Chaotic circuits; Chaotic oscillators; Delay dynamical systems; Hardware experiment; Multiscroll chaotic attractor; Numerical simulation; Phase portrait; Piece-wise linear functions; threshold controller; Time delayed, Circuit oscillations; Controllers; Operational amplifiers; Piecewise linear techniques, Chaotic systems.

http://arxiv.org/abs/1008.4011

www.worldscientific.com/doi/pdf/10.1142/S0218127411028751

DOI: 10.1142/S0218127411028751

85. Aridaman Pandit., **Somdatta Sinha (2011)** *Differential trends in the codon usage patterns in HIV-1 genes.* **PLoS ONE vol 6(12) e28889.**

ABSTRACT: Host-pathogen interactions underlie one of the most complex evolutionary phenomena resulting in continual adaptive genetic changes, where pathogens exploit the host's molecular resources for growth and survival, while hosts try to eliminate the pathogen. Deciphering the molecular basis of host–pathogen interactions is useful in understanding the factors governing pathogen evolution and disease propagation. In host-pathogen context, a balance between mutation, selection, and genetic drift is known to maintain codon bias in both organisms. Studies revealing determinants of the bias and its dynamics are central to the understanding of host-pathogen evolution. We considered the Human Immunodeficiency Virus (HIV) type 1 and its human host to search for evolutionary signatures in the viral genome. Positive selection is known to dominate intra-host evolution of HIV-1, whereas high genetic variability underlies the belief that neutral processes drive inter-host differences. In this study, we analyze the codon usage patterns of HIV-1 genomes across all subtypes and clades sequenced over a period of 23 years. We show presence of unique temporal correlations in the codon bias of three HIV-1 genes illustrating differential adaptation of the HIV-1 genes towards the host preferred codons. Our results point towards gene-specific translational selection to be an important force driving the evolution of HIV-1 at the population level.

http://www.plosone.org/article/info%3Adoi%2F10.1371%2Fjournal.pone.0028889

doi:10.1371/journal.pone.0028889

86. Kamal P. Singh., Sudeshna Sinha (2011) E*nhancement of "logical" responses by noise in a bistable optical system* .**Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 83 (4), art. no. 046219 .**

ABSTRACT: We verify numerically the phenomenon of logical stochastic resonance in a polarization bistable laser. Namely, we show that when one presents two weak binary inputs to the laser system, the response mirrors a logical or(nor) output. The reliability of the logic operation is dependent on the noise intensity. As one increases the noise, the probability of the output reflecting the desired or(nor) operation increases to nearly unity and then decreases. We also demonstrate that changing the bias morphs the output into another logic operation, and(nand), whose probability displays analogous behavior. Furthermore, we highlight the possibility of processing two logic gates in parallel in our laser system by exploiting two coupled orthogonal polarizations that can be detected simultaneously. This suggests that the computational power of the optical system may be enhanced by this additional potential for parallel processing. © 2011 American Physical Society.

KEYWORDS: Binary inputs; Bistable lasers; Bistable optical systems; Computational power; Laser systems; Logic operations; Noise intensities; Orthogonal polarizations; Parallel processing; Stochastic resonances, Magnetic resonance; Mirrors; Polarization, Optical systems

http://pre.aps.org/abstract/PRE/v83/i4/e046219

DOI: 10.1103/PhysRevE.83.046219

87. Nabi Hasan., **Visakhi.P (2011)** *e-Reading devices, products and services : Current Scenario and Future trends* : **Indian Journal of Agricultural Library and Information Services, Vol. 27(2) Jan-June : 71 -78p**

ABSTRACT: The paper covers the current scenario in new generation eReading devices especially touch eBooks and eReaders. It explores the digital world with some interesting data. The formats and technology of eBoooks and ebook readers have been narrated. The comparison of eBook vs Print books vs eReadres intermediary-Print on demand-has been explained. It further explores the business models and the benefits of buying eBooks through the aggregated eBook platform. eBook subscription issues for librarians have been listed. Next generation reading devices and the new utilities in reading through the machines have been explained. It further covers the transition from B2B to BC2C model. Cloud computing applications and digital content delivery for eBooks have been explored. Five laws of the library science in view of the development in the eReading environment have been re-interpreted. The authors see that the issue of new generation eReading devices is gaining momentum and the coming years would be interesting in exploring this interesting digital world

88. **R.Sengupta., Arvind (2011)** *Extremal extensions of entanglement witnesses: Finding new bound entangled states .* Physical Review A - Atomic, Molecular, and Optical Physics, 84 (3), art. no. 032328, .

ABSTRACT: In this paper, we discuss extremal extensions of entanglement witnesses based on Choi's map. The constructions are based on a generalization of the Choi map, from which we construct entanglement witnesses. These extremal extensions are powerful in terms of their capacity to detect entanglement of positive under partial transpose (PPT) entangled states and lead to unearthing of entanglement of new PPT states. We also use the Cholesky-like decomposition to construct entangled states which are revealed by these extremal entanglement witnesses. © 2011 American Physical Society.

KEYWORDS: Bound entangled state; Choi map; Entangled state; Entanglement witness; Extremal; Partial transpose, Quantum entanglement.

http://pra.aps.org/abstract/PRA/v84/i3/e032328

DOI:10.1103/PhysRevA.84.032328

89. Neal S. Gupta., Roger E. Summons **(2011)** *Fate of chitinous organisms in the geosphere*, **In : Topics in Geobiology 34 133-152. (Chapter 7)**

ABSTARCAT : Organic tissues such as cuticles may survive as organic remains and account for the fossil record of a number of important groups such as graptolites, chelicerates, insects, chitinozoans, ammonite beaks and fish scales. Fossilized cuticles were assumed to be composed of chitin protein complex similar to the living relatives, however, analysis of fossils using a range of mass spectrometric and spectroscopic methods have shown that preserved cuticles include significant amounts of aliphatic hydrocarbon component at times with an aromatic component that is very different to the composition of the cuticle of the living arthropod. Analysis of successively older fossil material has revealed that this transformation to an aliphatic composition is gradual and perhaps time dependant. Taphanomic incubation experiments demonstrate that lipids such as fatty acids are incorporated into the decaying chitin protein exoskeleton as early as a few weeks contributing to the aliphatic component. This is supported by chemolytic analysis of fossils that reveal presence of fatty acyl moieties in the macromolecule. Thus, the aliphatic composition in the fossils is generated in-situ and not from migration from an external source. Many kerogens are similarly

aliphatic and serve as a source for petroleum during thermal maturation. In such sedimentary organic matter where the contributing organism does not have a resistant aliphatic biopolymer, in situ lipid incorporation is likely an important mechanism for presence of the aliphatic component in the fossil organic matte

http://link.springer.com/chapter/10.1007%2F978-90-481-9684-5_7

DOI:10.1007/978-90-481-9684-5_7

90. Sourav Mitra., Girish Kulkarni., **J. S. Bagla.**, Jaswant K. Yadav **(2011)** *Formation rates of dark matter haloes* . **Bulletin of the Astronomical Society of India, 39 (4), pp. 1-30**

ABSTRACT: We derive an estimate of the rate of formation of dark matter haloes per unit volume as a function of the halo mass and redshift of formation. Analytical estimates of the number density of dark matter haloes are useful in modeling several cosmological phenomena. We use the excursion set formalism for computing the formation rate of dark matter haloes. We use an approach that allows us to differentiate between major and minor mergers, as this is a pertinent issue for semi-analytic models of galaxy formation. We compute the formation rate for the Press-Schechter and the Sheth-Tormen mass function. We show that the formation rate computed in this manner is positive at all scales. We comment on the Sasaki formalism where negative halo formation rates are obtained. Our estimates compare very well with N-body simulations for a variety of models. We also discuss the halo survival probability and the formation redshift distributions using our method.

KEYWORDS: Cosmology; Evolution - galaxies; Formation - galaxies; Haloes; Large scale structure of the universe - galaxies

http://arxiv.org/abs/1103.5828

http://connection.ebscohost.com/c/articles/85514268/formation-rates-dark-matter-haloes

91. Debmalya Roy., B. Shastri., C. N. Ramachandran., B. K. Mishra., K. Mukhopadhyay., **N. Sathyamurthy** and K. U. Bhasker Rao (**2011**) *Germanium encaged fullerene- synthesis, extraction, theoretical calculati**on and their possible application*** ***In*** : Germanium:**Properties, Production and Applications, Editor: Regina V. Germanno., Nova Science Publishers, Inc.** pp. 151-185

BookDescription: Germanium is an important semiconductor material used in transistors and various other electronic devices. Its major end uses are fiber-optic systems and infrared optics, but it is also used for polymerization catalysts, as well as in electronics and solar cell applications. This book presents current research in the study of germanium, including properties and generation by irradiation of germanium point defects in Ge-doped silica; Germanium encaged fullerene-synthesis; research of silicon and germanium structures with films of oxides and fluoride rare earth elements and new generation germanium detectors for double beta decay searches. (Imprint: Nova Press)

https://www.novapublishers.com/catalog/product_info.php?products_id=15563

92. Prashant Ramesh Desai., Anil Thakur., Dwaipayan Ganguli., Sanjoy Paul., Joachim Morschhäuser., **Anand K. Bachhawat (2011)** *Glutathione utilization by Candida albicans requires a functional glutathione degradation (DUG) pathway and OPT7, an unusual member of the oligopeptide transporter family.* **Journal of Biological Chemistry, 286 (48), pp. 41183-41194.**

ABSTRACT: Candida albicans lacks the ability to survive within its mammalian host in the absence of endogenous glutathione biosynthesis. To examine the ability of this yeast to utilize exogenous glutathione, we exploited the organic sulfur auxotrophy of C. albicans met15Δ strains. We observed that glutathione is utilized efficiently by the alternative pathway of glutathione degradation (DUG pathway). The major oligopeptide transporters OPT1-OPT5 of C. albicans that were most similar to the known yeast glutathione transporters were not found to contribute to glutathione transport to any significant extent. A genomic library approach to identify the glutathione transporter of C. albicans yielded OPT7 as the primary glutathione transporter. Biochemical studies on OPT7 using radiolabeled GSH uptake revealed a K_m of 205 μM, indicating that it was a high affinity glutathione transporter. OPT7 is unusual in several aspects. It is the most remote member to known yeast glutathione transporters, lacks the two highly conserved cysteines in the family that are known to be crucial in trafficking, and also has the ability to take up tripeptides. The transporter was regulated by sulfur sources in the medium. OPT7 orthologues were prevalent among many pathogenic yeasts and fungi and formed a distinct cluster quite remote from the Saccharomyces cerevisiae HGT1 glutathione transporter cluster. In vivo experiments using a systemic model of candidiasis failed to detect expression of OPT7 in vivo, and strains disrupted either in the degradation (dug3Δ) or transport (opt7Δ) of glutathione failed to show a defect in virulence. © 2011 by The American Society for Biochemistry and Molecular Biology, Inc.

KEYWORDS: Albicans; Auxotrophy; Biochemical studies; Candida albicans; Genomic libraries; Glutathione biosynthesis; Glutathiones; High affinity; In-vivo; In-vivo experiments; Mammalian hosts; Oligopeptides; Organic sulfur; Orthologues; Pathogenic yeast; Sulfur source; Tri-peptides, Amino acids; Biochemistry; Candida; Degradation; Mammals; Sulfur; Yeast, Peptides, cysteine; fungal protein; glutathione; oligopeptide transporter 7; protein DUG; unclassified drug, amino acid sequence; animal experiment; animal model; animal tissue; article; binding affinity; biochemistry; Candida albicans; candidiasis; controlled study; degradation; fungal virulence; glutathione metabolism; in vivo study; isotope labeling; male; mouse; nonhuman; priority journal; protein expression; protein function; regulatory mechanism, Candida albicans; Fungal Proteins; Gene Expression Regulation, Fungal; Glutathione; Membrane Transport Proteins; Multigene Family; Saccharomyces cerevisiae

http://www.jbc.org/content/286/48/41183.full.pdf+html

doi:10.1074/jbc.M111.272377

93. Gianluca Giovannetti., **Sanjeev Kumar.,** Alessandro Stroppa., Jeroen van den Brink., Silvia Picozzi., Jose Lorenzana

(2011) *High-Tc ferroelectricity emerging from magnetic degeneracy in cupric oxide.* **Physical Review Letters, 106 (2), art. no. 026401, .**

ABSTRACT: Cupric oxide is multiferroic at unusually high temperatures. From density functional calculations we find that the low-T magnetic phase is

paraelectric, and the higher-T one is ferroelectric with a size and direction of polarization in good agreement with experiments. By mapping the ab initio results on to an effective spin model, we show that the system has a manifold of almost degenerate ground states. In the high-T magnetic state noncollinearity and inversion symmetry breaking stabilize each other via the Dzyaloshinskii-Moriya interaction. This leads to an unconventional mechanism for multiferroicity, with the particular property that nonmagnetic impurities enhance the effect. © 2011 American Physical Society.

KEYWORDS: Ab initio; Cupric oxide; Density-functional calculations; Dzyaloshinskii-Moriya interaction; High temperature; High-T; Inversion symmetry; Magnetic degeneracy; Magnetic phase; Magnetic state; Multiferroics; Non-collinearity; Non-magnetic impurities; Paraelectrics; Spin models, Ferroelectricity

http://prl.aps.org/abstract/PRL/v106/i2/e026401

DOI:10.1103/PhysRevLett.106.026401

94. Neal S. Gupta., George D. Cody (**2011**) *Identification and characterization of chitin in organisms,* **Topics in Geobiology 34, 117-132 .**

ABSTRACT: Model compound chitin and invertebrate cuticles were analysed using pyrolysis-gas chromatography-mass spectrometry, 13 C NMR and C-, N-, The part-I of this paper attempts to evaluate the coral reef research in india using bibliometric tools for the period 1900-2000.The data has been extracted from “Bibliography on Indian coral reefs”. It highlights research productivity by subjects,domains,institutions(research and academic) etc. the study examines authorship pattern,productivity on individual scientists and also identified the various countries participation. It analyzes the forms of communication, journals productivity and identified the criteria for selection of the core journals for library. Suggested to create a database on coral reefs and to develop marine science at national level that would facilitate easy use of all categories of people. and O-Xray Absorption Near Edge Structure (XANES) spectral imaging using Scanning Transmission X-ray Microscopy (STXM) to detect spectra that are characteristic of chitin. Acetylpyridones, acetamidofuran, 3-acetamido-5-

methylfuran and 3-acetamido-(2 and 4)-pyrones appear to be characteristic pyrolysis products for chitin. Pyrolysis products with ions of m/z 70, 154, 168, 194 likely derive from diketopiperazine structures and provide potential markers for proteins and peptides in which proline, alanine, valine, arginine and glycine are the dominant amino acids. The 13C NMR spectra of chitin reveals that amidyl methyl group resonates at 23 ppm, amidyl linked glyocosyl carbon resonates at 56 ppm, glucosyl secondary alcohols resonate between 62 and 84 ppm, and glycosidic carbon absorption is evident at ~105 ppm. The presence of protein in the arthropod cuticles is evident by resonance intensity associated with sp2 bonded carbon associated in unsaturated amino acids (e.g. phenyl alanine, tyrosine, and histidine) occurring at 116, 129, and 137 ppm. Additionally, the protein back bone methine carbon atoms are indicated by resonance intensity at 43 ppm. Additional broad resonance intensity in the 20–30 ppm range is derived both from aliphatic aminoacids (e.g. valine and leucine) as well as the fatty acids associated with the waxy cuticulin layer of the cuticle. High energy resolution C-, N-, and O-XANES spectra provide further functional group level characterization of the biomacromolecular assemblages at spatial scales on the order of 100's of nm. Combining the power of Solid state 13C NMR, pyrolysis with the micro-analytical capabilities of C-, N-, and O-XANES yields a formidable analytical approach towards detecting and quantitating the presence of chitin in complex biomacromolecular assemblages.

http://link.springer.com/chapter/10.1007%2F978-90-481-9684-5_6?LI=true

DOI:10.1007/978-90-481-9684-5_6

95. **Meera Nanda (2011)** *Ideological Convergences: Hindutva and the Norway Mas-sacre,* Economic and Political Weekly, Volume xlvi (53), pp. 61-68.

ABSTRACT : Anders Breivik, the man who carried out the July 2011 massacre in Norway, counts the sanatana dharma movements in India among his allies in Europe's supposed war against Islam. His manifesto refers to Koenraad Elst, a well-known Belgian critic of Islam who is also a strong votary of Hindutva in India. In addition, many other Indian writers are also quoted by Breivik. This essay looks at the shared world view, agenda and history of this school of Hindutva, and the anti-Islamic European right.

http://www.epw.in/special-articles/ideological-convergences-hindutva-and-norway-massacre.html

96. Neeraj Kumar Kamal., **Sudeshna Sinha (2011)** *Imbalance of positive and negative links induces regularity* . **Chaos, Solitons and Fractals, 44 (1-3), pp. 71-78.**

ABSTRACT: We investigate the effect of the interplay of positive and negative links, on the dynamical regularity of a random weighted network, with neuronal dynamics at the nodes. We investigate how the mean J and the variance of the weights of links, influence the spatiotemporal regularity of this dynamical network. We find that when the connections are predominantly positive (i.e. the links are mostly excitatory, with J>0) the spatiotemporal fixed point is stable. A similar trend is observed when the connections are predominantly negative (i.e. the links are mostly inhibitory, with J<0). However, when the positive and negative feedback is quite balanced (namely, when the mean of the connection weights is close to zero) one observes spatiotemporal chaos. That is, the balance of excitatory and inhibitory connections preserves the chaotic nature of the uncoupled case. To be brought to an inactive state one needs one type of connection (either excitatory or inhibitory) to dominate. Further we observe that larger network size leads to greater spatiotemporal regularity. We rationalize our observations through mean field analysis of the networkM. Karanam, S. Dev and A. R. Choudhury Crystal Growth & Design, 12(1), 240-252 (2012). dynamics. © 2010 Elsevier Ltd. All rights reserved.

KEYWORDS: Chaotic nature; Connection weights; Dynamical networks; Fixed points; Larger networks; Mean field analysis; Negative feedback; Network dynamics; Neuronal dynamics; Spatiotemporal chaos; Weighted networks, Feedback

http://www.sciencedirect.com/science/article/pii/S0960077910000263

http://dx.doi.org/10.1016

97. **Mily Bhattacharya., Neha Jain., Samrat Mukhopadhyay (2011)** *Insights into the mechanism of aggregation and fibril formation from bovine serum albumin*. **Journal of Physical Chemistry B, 115 (14), pp. 4195-4205.**

ABSTRACT: We have investigated the fibrillation propensity of different conformational isomers of an archetypal, all α-helical protein, namely, bovine serum albumin (BSA), under different pH conditions and ionic strengths using fluorescence and circular dichroism (CD) spectroscopy. At low pH and higher protein concentration, the partially folded conformers associate to form oligomers that are converted into ordered amyloid-like fibrils when incubated at elevated temperature. We have elucidated the mechanism of fibril formation, especially the early steps, by monitoring the kinetics of structural changes during the aggregation process. Various structural probes in tandem were utilized to decipher the temporal evolution of both conformational and size changes by measuring the time dependence of fluorescence intensity and anisotropy of intrinsic tryptophans and several extrinsic fluorophores during the aggregation. Additionally, CD spectroscopy was utilized to monitor the changes in protein secondary structural content during fibrillation. Our findings suggest that the conformational conversion occurs in the oligomers that serve as precursors to amyloid fibrils and precedes the overall fibrillar growth. © 2011 American Chemical Society.

KEYWORDS: Aggregation process; Amyloid fibril; Amyloid-like fibril; Bovine serum albumins; CD spectroscopy; Circular dichroism; Conformational conversion; Conformational isomers; Elevated temperature; Fibril formation; Fluorescence intensities; Helical proteins; Intrinsic tryptophans; pH condition; Protein concentrations; Structural change; Structural content; Structural probes; Temporal evolution; Time dependence, Agglomeration; Amino acids; Body fluids; Dichroism; Fluorophores; Glycoproteins; Ionic strength; Isomers; Oligomers; Proteins, Circular dichroism spectroscopy, amyloid; bovine serum albumin, animal; article; cattle; chemistry; circular dichroism; pH; protein secondary structure, Amyloid; Animals; Cattle; Circular Dichroism; Hydrogen-Ion Concentration; Protein Structure, Secondary; Serum Albumin, Bovine

http://pubs.acs.org/doi/abs/10.1021/jp111528c
DOI: 10.1021/jp111528c

98. **Dinesh Khurana.**, T. Y. Lam **(2011)** *Invertible commutators in matrix rings,* **J. Alg. Appl. 10 (1) pp.,51-71**

ABSTRACT: In a matrix ring $R = \mathbb{M}_2(S)$ where S is a commutative ring, we study equations of the form $XY - YX = U \in GL_2(S)$, focusing on matrices in R that can appear as X or as XY in such equations. These are the *completable* and the *reflectable* matrices in R. For matrices $A \in R$ with a zero row or with a constant diagonal, explicit and "computer-checkable" criteria are found for A to be completable or reflectable. A formula for det (XY - YX) discovered recently with Shomron connects this study to diophantine questions about the representation of units of the ground ring S by quadratic forms of the type $px^2 + qy^2$.

KEYWORDS: Matrix rings; additive commutators; completable and *reflectable matrices; determinantal formulas; binary quadratic forms.*

http://www.worldscientific.com/doi/abs/10.1142/S0219498811004422
DOI: 10.1142/S0219498811004422

99. Neha Jain., Mily Bhattacharya., Samrat Mukhopadhyay (2011) *Kinetics of surfactant-induced aggregation of lysozyme studied by fluorescence spectroscopy .* **Journal of Fluorescence, 21 (2), pp. 615-625.**

ABSTRACT: The study of protein conformational changes in the presence of surfactants and lipids is important in the context of protein folding and misfolding. In the present study, we have investigated the mechanism of the protein conformational change coupled with aggregation leading to size growth of Hen Egg White Lysozyme (HEWL) in the presence of an anionic detergent such as sodium dodecyl sulphate (SDS) in alkaline pH. We have utilized intrinsic protein fluorescence (tryptophan) and extrinsic fluorescent reporters such as 8-anilinonaphthalene-1- sulfonic acid (ANS), dansyl and fluorescein to follow the protein conformational change in realtime. By analyzing the kinetics of fluorescence intensity and anisotropy of multiple fluorescent reporters, we have been able to delineate the mechanism of surfactant-induced aggregation of lysozyme. The kinetic parameters reveal that aggregation proceeds with an initial fast-phase (conformational change) followed by a slow-phase (self-assembly). Our results indicate that SDS, below critical micelle concentration, induces conformational expansion that triggers the aggregation process at a micromolar protein concentration range. © 2010 Springer Science+Business Media, LLC.

KEYWORDS: Aggregation process; Alkaline pH; Anionic detergents; Conformational change; Fluorescence anisotropy; Fluorescence intensities; Fluorescent reporter; Hen egg white lysozyme; Intrinsic protein fluorescence; Lysozyme; Misfolding; Protein aggregation; Protein concentrations; Real time; Sodium dodecyl sulphate; Sulfonic acid, Alkalinity; Amino acids; Anisotropy; Critical micelle concentration; Dyes; Enzymes; Fluorescence; Fluorescence spectroscopy; Kinetics; Protein folding; Proteins; Sodium, Agglomeration, dodecyl sulfate sodium; fluorescent dye; lysozyme; surfactant, amino acid sequence; animal; article; chemical structure; chemistry; dose response; drug effect; kinetics; molecular genetics; pH; protein multimerization; protein quaternary structure; solubility; spectrofluorometry, Amino Acid Sequence; Animals; Dose-Response Relationship, Drug; Fluorescent Dyes; Hydrogen-Ion Concentration; Kinetics; Models, Molecular; Molecular Sequence Data; Muramidase; Protein Multimerization; Protein Structure, Quaternary; Sodium Dodecyl Sulfate; Solubility; Spectrometry, Fluorescence; Surface-Active Agents

http://link.springer.com/article/10.1007%2Fs10895-010-0749-3#page-1

DOI 10.1007/s10895-010-0749-3

100. X. Liu., T. Berlijn., W.-G. Yin., W. Ku, A. Tsvelik., Young-June Kim., H. Gretarsson., **Yogesh Singh.**, P. Gegenwart, J. P. Hill (**2011**) *Long-range magnetic ordering in Na_2IrO_3.* **Physical Review B - Condensed Matter and Materials Physics, 83 (22), art. no. 220403, .**

ABSTRACT: We report a combined experimental and theoretical investigation of the magnetic structure of the honeycomb-lattice magnet Na_2IrO_3, a candidate for a realization of a gapless spin liquid. Using resonant x-ray magnetic scattering at the Ir L_3 edge, we find three-dimensional long-range antiferromagnetic order below T_N=13.3 K. From the azimuthal dependence of the magnetic Bragg peak, the ordered moment is determined to be predominantly along the a axis. Combining the experimental data with first-principles calculations, we propose that the most likely spin structure is a zig-zag structure. © 2011 American Physical Society.

http://prb.aps.org/abstract/PRB/v83/i22/e220403

DOI: 10.1103/PhysRevB.83.220403

101. Jorn W. F. Venderbos., Maria Daghofer., Jeroen van den Brink., **Sanjeev Kumar** (**2011**) *Macroscopic Degeneracy and Emergent Frustration in a Honeycomb Lattice Magnet* . **Physical Review Letters, 107 (7), art. no. 076405, .**

ABSTRACT: Using a hybrid method based on fermionic diagonalization and classical Monte Carlo techniques, we investigate the interplay between itinerant and localized spins, with competing double- and superexchange interactions, on a honeycomb lattice. For moderate superexchange, a geometrically frustrated triangular lattice of hexagons forms spontaneously. For slightly larger superexchange a dimerized ground state is stable that has macroscopic degeneracy. The presence of these states on a nonfrustrated honeycomb lattice highlights novel phenomena in this itinerant electron system: emergent geometrical frustration and degeneracy related to a symmetry intermediate between local and global. © 2011 American Physical Society.

KEYWORDS: Diagonalizations; Geometrical frustrations; Honeycomb lattices; Hybrid method; Itinerant electron system; Localized spin; Monte Carlo techniques; Superexchange interaction; Superexchanges; Triangular lattice, Monte Carlo methods, Honeycomb structures

http://prl.aps.org/abstract/PRL/v107/i7/e076405

DOI:10.1103/PhysRevLett.107.076405

102. Bindiya Arora., M. S. Safronova., Charles W. Clark (**2011**) *Magic-zero wave- lengths for alkali atoms and their applications*, **Phys. Rev. A 84, 043401**

ABSTRACT : Using first-principles calculations, we identify "magic-zero" optical wavelengths, λzero , for which the ground-state frequency-dependent polarizabilities of alkali-metal atoms vanish. Our approach uses high-precision, relativistic all-order methods in which all single, double, and partial triple excitations of the Dirac-Fock wave functions are included to all orders of perturbation theory. We discuss the use of magic-zero wavelengths for sympathetic cooling in two-species mixtures of alkalis with group-II and other elements of interest. Special cases in which these wavelengths coincide withstrong resonance transitions in a target system are identified.

http://arxiv.org/abs/1107.206

http://meetings.aps.org/Meeting/DAMOP11/Event/147422

103. Ajay Pal Singh Pannu., Pratibha Kapoor., Geeta Hundal., **Ramesh Kapoor.,** Montserrat Corbella., Núria Aliaga-Alcalde., Maninder Singh Hundal. **(2011)** *Magneto-structural studies of two new cobalt(ii)-N,N-diisobutylisonicotinamide compounds: $[CoLCl_2]_n$ and $[Co(L)_2(H_2O)_4][CoLBr_3]_2{\cdot}2H_2O$* **Dalton Transactions, 40 (46), pp. 12560-12569.**

ABSTRACT: Two similar synthetic pathways using the ligand N,N-diisobutylisonicotinamide (L) with anhydrous CoX_2 salts (being X = Cl^-, Br^-) led to different species: a one-dimensional system, $[CoLCl_2]_n$, 1, and an ionic product $[Co(L)_2(H_2O)_4][CoLBr_3]_2\cdot 2H_2O$,2,respectively. Compound 1 is a polymer in which ligand L coordinates to tetrahedral Co ^{II} ions in a bidentate bridging fashion using the pyridine nitrogen and carbonyl oxygen atoms. Compound 2 consists of one octahedral cationic $[Co(L)_2(H_2O)_4]^{2+}$ entity and two tetrahedral anionic $[CoLBr_3]^-$ units. In this system, the ligand molecules coordinate only through the pyridine nitrogen atoms. The magnetic properties of 1 and 2 were investigated in the temperature range of 2.0 to 300.0 K and correlations between both (due to the existence of similar features) examined. The study of the magnetic properties of 1 was carried out by considering each Co ^{II} ion as a perfectly isolated system, hence, J = 0, but taking into account a significant zero-field splitting contribution due to distortions on the tetrahedral environment of the cobalt atoms. The fit of the magnetic susceptibility data together with reduced magnetization vs H/T measurements provided similar parameters (D = 10.8 cm $^{-1}$, g_1 = 1.92, g_1 = 2.92 for the former and D = 11.04 cm $^{-1}$and g = 2.05 for the latter, respectively). On the other hand, the magnetic response of compound 2 has been analyzed using a model which considers the presence of two tetrahedral and one octahedral Co(ii) ions (Co $_{Td}$ and Co $_{Oh)}$. The study was carried out in two separated blocks, above and below 80 K, where only the most significant effects at each interval of temperature were considered. As a result, the analysis of the magnetic data shows weak antiferromagnetic interactions between the Co $_{Oh}$and the two Co $_{Td}$ ions (J = -0.41 cm $^{-1)}$ in 2. The best fit parameters were g $_{CoTd}$ = 2.89, g $_{CoOh}$ = 3.50, $_{D\ CoTd}$ = 10.62 cm $^{-1}$, E $_{CoTd}$ = 2.95 cm $^{-1,}$ Δ = 240.9 cm $^{-1}$ and J $_{L-S}$ = -107.1 cm $^{-1,}$ from where λ was calculated with a final value of -144.8 cm $^{-1}$ (J $_{L-S}$ = $A_{\kappa\lambda}$). The approximations performed to obtain these values provide reasonable results in agreement with compound 1 and also to other systems in the literature. This journal is © The Royal Society of Chemistry.

KEYWORDS: Antiferro-magnetic interactions; Best fit; Carbonyl oxygen atoms; Cobalt atoms; Ionic products; Isolated systems; Ligand molecules; Magnetic data; Magnetic response; One-dimensional systems; Pyridine nitrogen; Pyridine-nitrogen atom; Synthetic pathways; Temperature range; Zero-field splittings, Antiferromagnetism; Atoms; Bromine compounds; Carbonyl compounds; Chlorine compounds; Cobalt; Ions; Ligands; Magnetic susceptibility; Pyridine, Cobalt compounds

http://pubs.rsc.org/en/Content/ArticleLanding/2011/DT/c1dt10991j

DOI:10.1039/C1DT10991J

104. Stéphanie Bedhomme., Adam K. Chippindale., **N. G. Prasad.,** Matthieu Delcourt., Jessica K. Abbott1., Martin A. Mallet., Howard D. Rundle **(2011)** *Male-limited evolution suggests no extant intralocus sexual conflict over the sexually dimorphic cuticular hydrocarbons of Drosophila melanogaster.* **Journal of Genetics, 90 (3), pp. 443-452.**

ABSTRACT: Sexually dimorphic traits are likely to have evolved through sexually antagonistic selection. However, recent empirical data suggest that intralocus sexual conflict often persists, even when traits have diverged between males and females. This implies that evolved dimorphism is often incomplete in resolving intralocus conflict, providing a mechanism for the maintenance of genetic variance in fitness-related traits. We used experimental evolution in Drosophila melanogaster to directly test for ongoing conflict over a suite of sexually dimorphic cuticular hydrocarbons (CHCs) that are likely targets of sex-specific selection. Using a set of experimental populations in which the transmission of genetic material had been restricted to males for 82 generations, we show that CHCs did not evolve, providing experimental evidence for the absence of current intralocus sexual conflict over these traits. The absence of ongoing conflict could indicate that CHCs have never been the target of sexually antagonistic selection, although this would require the existing dimorphism to have evolved via completely sex-linked mutations or as a result of former, but now absent, pleiotropic effects of the underlying loci on another trait under sexually antagonistic selection. An alternative interpretation, and which we believe to be more likely, is that the extensive CHC sexual dimorphism is the result of past intralocus sexual conflict that has been fully resolved, implying that these traits have evolved genetic independence between the sexes and that genetic variation in them is therefore maintained by alternative mechanisms. This latter interpretation is consistent with the known roles of CHCs in sexual communication in this species and with previous studies suggesting the genetic independence of CHCs between males and females. Nevertheless, direct estimates of sexually antagonistic selection will be important to fully resolve these alternatives. © 2011 Indian Academy of Sciences.

KEYWORDS: cuticular hydrocarbons; Drosophila melanogaster; experimental evolution; intralocus sexual conflict; male-limited evolution; sexual dimorphism

www.ias.ac.in/jgenet/Vol90No3/443.pdf

105. K. Imroze., **N. G. Prasad** **(2011)** *Mating with large males decreases the immune defence of females in Drosophila melanogaster*. **Journal of Genetics, 90 (3), pp. 427-434.**

ABSTRACT: Mating has been widely reported to be a costly event for females. Studies indicate that female cost of mating in terms of fecundity and survivorship can be affected by their mates, leading to antagonistic coevolution between the sexes. However, as of now, there is no evidence that the female cost of mating in terms of immune defence is affected by their mates. We assess the effect of different sized males on antibacterial immune defence and reproductive fitness of their mates. We used a large outbred population of Drososphila melanogaster as the host and Serratia marcescens as the pathogen. We generated three different male phenotypes: small, medium and large, by manipulating larval densities. Compared to females mating with small males, those mating with large males had higher bacterial loads and lower fecundity. There was no significant effect of male phenotype on the fraction of females mated or copulation duration (an indicator of ejaculate investment). Thus, our study is the first clear demonstration that male phenotype can affect the cost of mating to females in terms of their antibacterial immune defence. Mating with large males imposes an additional cost of mating to females in terms of reduced immune defence. The observed results are very likely due to qualitative/quantitative differences in the ejaculates of the three different types of males. If the phenotypic variation that we observed in males in our study is mirrored by genetic variation, then, it can potentially lead to antagonistic coevolution of the sexes over immune defence. © 2011 Indian Academy of Sciences.

KEYWORDS: Bacteria (microorganisms); Drosophila melanogaster; Melanogaster; Serratia marcescens, animal; article; bacterial load; body size; Drosophila melanogaster; female; fertility; immunology; larva; male; microbiology; pathogenicity; phenotype; physiology; Serratia marcescens; sexual behavior; time, Animals; Bacterial Load; Body Size; Drosophila melanogaster; Female; Fertility; Larva; Male; Phenotype; Serratia marcescens; Sexual Behavior, Animal; Time Factors

www.ias.ac.in/jgenet/Vol90No3/427.pdf

106. Sudip Mandal., Anne G. Lindgren., Anand S. Srivastava., Amander T. Clark., Utpal Banerjee **(2011)** *Mitochondrial function controls proliferation and early differentiation potential of embryonic stem cells* . **Stem Cells, 29 (3), pp. 486-495.**

ABSTRACT: Pluripotent stem cells hold significant promise in regenerative medicine due to their unlimited capacity for self-renewal and potential to differentiate into any cell type of the body. In this study, we demonstrate that proper mitochondrial function is essential for proliferation of undifferentiated ESCs. Attenuating mitochondrial function under self-renewing conditions makes these cells more glycolytic-dependent, and it is associated with an increase in the mRNA reserves of Nanog, Oct4, and Sox2. In contrast, attenuating mitochondrial function during the first 7 days of differentiation results in normal repression of Oct4, Nanog, and Sox2. However, differentiation potential is compromised as revealed by abnormal transcription of multiple Hox genes. Furthermore, under differentiating conditions in which mitochondrial function is attenuated, tumorigenic cells continue to persist. Our results, therefore establish the importance of normal mitochondrial function in ESC proliferation, regulating differentiation, and preventing the emergence of tumorigenic cells during the process of differentiation. © AlphaMed Press.

KEYWORDS: messenger RNA; octamer transcription factor 4; transcription factor NANOG; transcription factor Sox2, animal cell; animal tissue; article; carcinogenesis; cell differentiation; cell function; cell proliferation; controlled study; embryonic stem cell; genetic transcription; glycolysis; human; human cell; human tissue; mitochondrion; mouse; nonhuman, Animals; Cell Culture Techniques; Cell Differentiation; Cell Proliferation; Cells, Cultured; Embryonic Stem Cells; Gene Expression Regulation, Developmental; Humans; Male; Mice; Mice, SCID; Mitochondria; Pluripotent Stem Cells; Time Factors

http://onlinelibrary.wiley.com/doi/10.1002/stem.590/pdf

DOI: 10.1002/stem.590

107. D.Mogensen., S.Smolander., A.Sogachev., L.Zhou., **V. Sinha.,** A.Guenther, J.Williams, T.Nieminen, M.K.Kajos, J.Rinne, M.Kulmala., M.Boy **(2011)** *Modelling atmospheric OH-reactivity in a boreal forest ecosystem,* **Atmos. Chem. Phys., 11, pp.,9709-9719**

ABSTRACT: We have modelled the total atmospheric OH- reactivity in a boreal forest and investigated the individ- ual contributions from gas phase inorganic species, iso- prene, monoterpenes, and methane along with other impor- tant VOCs. Daily and seasonal variation in OH-reactivity for the year 2008 was examined as well as the vertical OH- reactivity profile. We have used SOSA; a one dimensional vertical chemistry-transport model (Boy et al., 2011a) to- gether with measurements from Hyyti¨ l¨ , SMEAR II station, aa Southern Finland, conducted in August 2008. Model sim- ulations only account for ~30–50 % of the total measured OH sink, and in our opinion, the reason for missing OH-reactivity is due to unmeasured unknown BVOCs, and limi- tations in our knowledge of atmospheric chemistry including uncertainties in rate constants. Furthermore, we found that the OH-reactivity correlates with both organic and inorganic compounds and increases during summer. The summertime canopy level OH-reactivity peaks during night and the verti- cal OH-reactivity decreases with height.

http://www.atmos-chem-phys.net/11/9709/2011/acp-11-9709-2011.html

doi:10.5194/acp-11-9709-2011

108. *Animesh Gupta., Aman Sohane.,* ***Vivek Kohar.****, K. Murali.,* ***Sudeshna Sinha.*****, (2011)** Noise-free logical stochastic resonance . **Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 84 (5), art. no. 055201, .**

ABSTRACT: The phenomena of logical stochastic resonance (LSR) was demonstrated recently: namely, when a bistable system is driven by two inputs it consistently yields a response mirroring a logic function of the two inputs in an optimal window of moderate noise. Here we examine the intriguing possibility of obtaining dynamical behavior equivalent to LSR in a noise-free bistable system, subjected only to periodic forcing, such as sinusoidal driving or rectangular pulse trains. We find that such a system, despite having no stochastic influence, also yields phenomena analogous to LSR, in an appropriate window of frequency and amplitude of the periodic forcing. The results are corroborated by circuit experiments. © 2011 American Physical Society.

KEYWORDS: Bistable system; Circuit experiments; Dynamical behaviors; Logic functions; Periodic forcing; Rectangular pulse; Sinusoidal driving; Stochastic resonances, Circuit resonance; Magnetic resonance, Stochastic systems

http://pre.aps.org/abstract/PRE/v84/i5/e055201

DOI: 10.1103/PhysRevE.84.055201

109. K. Murali., **Sudeshna Sinha.,** Adi R. Bulsara., Anna Dari., William L. Ditto (**2011)** *Noise Enhanced Logic Gates*, **AIP Conf. Proc. 1339, pp. 67-77 .**

ABSTRACT: It was observed recently that, when one drives a two-state system with two square wave as input, the response of the system mirrors a logical output (NOR/OR). The probability of obtaining the correct logic response is controlled by the interplay between the noise-floor and the nonlinearity. As one increases the noise intensity, the probability of the output reflecting a NOR/OR operation increases to unity in a window of moderate noise, and then decreases to zero again for very large noise. This concept of noise enhanced logic gate performance under optimal noise was called: Logical Stochastic Resonance (LSR). Here we review this concept of Logical Stochastic Resonance and provide details of suitable electronic circuit systems demonstrating LSR. We also review the extension of this approach to realize logic gates with Coherence Resonance Systems (LCR).

http://proceedings.aip.org/resource/2/apcpcs/1339/1/67_1?isAuthorized=no

doi:http://dx.doi.org/10.1063/1.3574845

110. Krishnendu Gongopadhyay., Ravi S. Kulkarni (**2011**) *On the existence of an invariant non-degenerate bilinear form under a linear map* . **Linear Algebra and Its Applications, 434 (1), pp. 89-103.**

ABSTRACT: Let V be a vector space over a field F. Assume that the characteristic of F is large, i.e. char(F)>dimV. Let T:V→V be an invertible linear map. We answer the following question in this paper. When does V admit a T-invariant non-degenerate symmetric (resp. skew-symmetric) bilinear form? We also answer the infinitesimal version of this question. Following Feit and Zuckerman 2, an element g in a group G is called real if it is conjugate in G to its own inverse. So it is important to characterize real elements in GL(V,F). As a consequence of the answers to the above question, we offer a characterization of the real elements in GL(V,F). Suppose V is equipped with a non-degenerate symmetric (resp. skew-symmetric) bilinear form B. Let S be an element in the isometry group I(V,B). A non-degenerate S-invariant subspace W of (V,B) is called orthogonally indecomposable with respect to S if it is not an orthogonal sum of proper S-invariant subspaces. We classify the orthogonally indecomposable subspaces. This problem is non-trivial for the unipotent elements in I(V,B). The level of a unipotent T is the least integer k such that (T-I)k=0. We also classify the levels of unipotents in I(V,B). © 2010 Elsevier Inc. All rights reserved.

KEYWORDS: Bilinear form; Linear maps; Non-trivial; Orthogonal sum; Real elements; S-invariant; Skew-symmetric; T-invariant; Unipotents, Vector spaces, Vectors

http://arxiv.org/abs/0903.0826

http://www.sciencedirect.com/science/article/pii/S0024379510004179

111. Manoj Kumar Pandey., Ramesh Ramachandran (**2011**) *Operator-based analytic theory of decoherence in NMR* . **Molecular Physics, 109 (12), pp. 1545-1565.**

ABSTRACT: The operator-based analytic description of polarization transfer in NMR spectroscopy is often fraught with difficulty due to (a) the dimension and (b) the non-commuting nature of the spin Hamiltonians. In this article, an analytic model is presented to elucidate the mechanism of polarization transfer between dilute spins I_1 and I_2 coupled to a reservoir of abundant S-spins (i.e. $[I_1 - I_2]S_N$) in the solid state. Specifically, the factors responsible for the decoherence observed in double cross-polarization (DCP) experiments are outlined in terms of operators via effective Floquet Hamiltonians. The interplay between the various anisotropic interactions is thoroughly investigated by comparing the simulations from the analytic theory with exact numerical methods. The analytical theory presents a framework for incorporating multi-spin effects within a reduced subspace spanned by spinsI_1 and I_2. The simulation results from the analytic model comprising eight spins are in excellent agreement with the numerical methods and present an attractive tool for understanding the phenomenon of decoherence in NMR. © 2011 Taylor & Francis.

KEYWORDS: Analytic models; Analytic theory; Analytical theory; Anisotropic interaction; Cross polarizations; Decoherence; Effective Hamiltonian; Floquet Hamiltonian; Polarization transfer; Simulation result; Spin Hamiltonian, Computer simulation; Hamiltonians; Nuclear magnetic resonance spectroscopy; Numerical methods; Polarization, Quantum theory

http://www.tandfonline.com/doi/abs/10.1080/00268976.2011.572088

DOI:10.1080/00268976.2011.572088

112. Kausik Chattopadhyay (2011) *Overview of protein molecular structures: Implications for functions* In: **Fundamentals and Current Topics in Molecular Structure Research**, p115-146 [ISBN: 978-81-308-0458-3; Research Signpost, India].

ABSTRACT: Proteins are one of the most important classes of macromolecules implicated in diverse critical biological processes. Each individual protein molecule is composed of a unique amino acid sequence encoded by the genome of the given organism. Based on its unique amino acid sequence, each protein molecule adopts a definite three-dimensional structure that ultimately dictates the functionality of the given protein. Toward elucidating this ‘protein structure-function paradigm’, the present discussion attempts to highlight some of the salient features of the protein molecular structures with special emphasis on some of the prominent protein structural folds, families, and superfamilies.

http://www.ressign.com/UserArticleDetails.aspx?arid=11029

113. Mily Bhattacharya., Neha Jain, Karishma Bhasne., Vandna Kumari., Samrat Mukhopadhyay (2011) P*H-Induced conformational isomerization of bovine serum albumin studied by extrinsic and intrinsic protein fluorescence*. **Journal of Fluorescence, 21 (3), pp. 1083-1090.**

ABSTRACT: Serum albumins are multi-domain all α-helical proteins that are present in the circulatory system and aid in the transport of a variety of metabolites, endogenous ligands, drugs etc. Earlier observations have indicated that serum albumins adopt a range of reversible conformational isomers depending on the pH of the solution. Herein, we report the concurrent changes in the protein conformation and size that are inherent to the pH-induced conformational isomers of bovine serum albumin (BSA). We have investigated the fluorescence properties of both intrinsic (tryptophan) and extrinsic (ANS, pyrene) fluorophores to shed light into the structural features of the pH-dependent conformers. We have been able to identify a number of conformational isomers using multiple fluorescence observables as a function of pH titration. Our results indicate that at pH 3, a partially-folded, 'molten-globule-like' state is populated. Moreover, equilibrium unfolding studies indicated that the 'molten-globule-like' state unfolds in a non-cooperative fashion and is thermodynamically less stable than the native state. The fluorescence-based approach described in the present work has implications in the study of pH-induced conformational plasticity of other physiologically relevant proteins. © Springer Science+Business Media, LLC 2011.

KEYWORDS: Bovine serum albumins; Circulatory systems; Conformational isomerization; Conformational isomers; Conformational plasticity; Fluorescence anisotropy; Fluorescence properties; Helical proteins; Intrinsic protein fluorescence; Molten-globule; Multi domains; Native state; Non-cooperative; PH titration; PH-dependent; Protein conformation; Serum albumin; Structural feature, Amino acids; Cardiovascular system; Fluorescence; Fluorescence spectroscopy; Fluorophores; Isomers; Proteins, Body fluids, 8 anilino 1 naphthalenesulfonic acid; bovine serum albumin; tryptophan, chemistry; conference paper; fluorescence; isomerism; pH; protein conformation; protein folding, Anilino Naphthalenesulfonates; Fluorescence; Hydrogen-Ion Concentration; Isomerism; Protein Conformation; Protein Folding; Serum Albumin, Bovine; Tryptophan, Bovinae

http://link.springer.com/article/10.1007%2Fs10895-010-0781-3?LI=true#page-1

DOI:10.1007/s10895-010-0781-3

114. Ram Dulare., M.K.Bharty., S.K.Kushawaha., **Sanjay Singh.**, N.K. Singh **(2011)** *Polymeric Hg(II) and dimeric oxo-bridged manganese(II) complexes derived from N′-(2-methyl-benzoyl)-hydrazinecarbodithioic acid methyl ester: Synthesis, spectral and structural characterization.* **Polyhedron, 30 (12), pp. 1960-1967.**

ABSTRACT: Reaction of N′-(2-methyl-benzoyl)-hydrazinecarbodithioic acid methyl ester (H_2mbhe) with $HgCl_2$ and $Mn(OAc)_2$. $4H_2O$ yielded the polymeric $[Hg_3(tot)_2(\mu\text{-}SCH_{3)}{}_{4]}{}_{n}$ (1) and dimeric $[Mn_2(Hmbhe)_2(\mu\text{-}mbmst)_2]$ $CHCl_3$ (2), respectively. These complexes have been synthesized and their structures investigated by elemental analyses, NMR, IR, UV-Vis and single crystal X-ray data. In one unit of the polymeric structure of complex 1, two Hg(II) are similar bonded to an exocyclic sulfur of oxadiazole and three sulfur of SCH_3 whereas one Hg(II) is two coordinate linked to two SCH_3 fragments. Thus, complex 1 shows the presence of tetrahedral as well as linear Hg(II) in the same molecule. The dimeric octahedral complex 2 contains thiadiazolyl hydrazide moiety (mbmst) formed from H_2mbhe under thermal condition which is bonded in a tetradentate manner by two nitrogens and one bidentate bridged oxygen between two Mn(II) centers. In the solid state both complexes are stabilized by intermolecular hydrogen bonding and form supramolecular architecture. © 2011 Elsevier Ltd.

KEYWORDS: 1,3,4-Oxadiazole; 1,3,4-Thiadiazolyl hydrazide; Dimeric oxo-bridge Mn(II) complex; Four and two coordinate Hg(II) complex; Supramolecular architecture

http://www.sciencedirect.com/science/article/pii/S0277538711002786

115. Amit Kulshrestha., Anupam Singh **(2011)** *Real Elements and Schur Indices of a Group*, **Mathematics Student 80, pp. 73-84**

ABSTRACT : In this article we try to explore the relation between real conjugacy classes and real characters of finite groups at more refined level. This refinement is in terms of properties of groups such as strong reality and total orthogonality. In this connection we raise several questions and record several examples which have motivated those questions.

KEYWORDS: Real Elements ; Schur Indices;a Group

http://arxiv.org/abs/1104.3933

116. Zhou Wang., Jianlong Chen., **Dinesh Khurana.,** Tsit-Yuen Lam **(2011)** *Rings of Idem- potent Stable Range One,* **Algebras and Representation Theory.,** 15,(1) pp 195-200

ABSTRACT: : We show that in a ring of stable range 1, any (von Neumann) regular element is clean. Our main results also imply that any unit-regular ring has idempotent stable range 1 (and is therefore clean), and that a semilocal ring has idempotent stable range 1 if and only if it is semiperfect.

KEYWORDS : Idempotent stable range one · Stable range one · Regular elements· Unit regular rings· Clean rings

http://link.springer.com/article/10.1007%2Fs10468-011-9276-4
DOI 10.1007/s10468-011-9276-4

117. K. Koteswara Rao (2011) Reproduction and Transmission of Knowledge in*Tribal Societies: A Study among Konda Reddis of Eastern Ghats in Andhra Pradesh*. **Humankind (Serials Publications), Vol. 7, pp. 101-110.**

ABSTRCAT: Reproduction and transmission of knowledge are as important as theknowledge itself. They are vital in the cultural production of knowledge and for cultural continuity. Knowledge in traditional societies is culturally reproduced and transmitted across generations as a continuous process. This determines the state of the knowledge as well as the society. The present paper, therefore, tries to understand the role of transmission and reproduction of knowledge among tribal societies with reference to the Konda Reddis. The paper analyzes how the processes of transmission and reproduction, stock of the knowledge, and state of the society are interrelated and influence one another.

KEYWORDS: traditional knowledge, ethnobotanical knowledge, knowledge transmission, knowledge acquisition, Konda Reddis.

http://www.serialspublications.com/contentnormal.asp?jid=402&jtype=1

118. B. Nandy., N.G.Prasad (2011) *Reproductive behavior and fitness components in male Drosophila melaogaster are non-linearly affected by the number of male co-inhabitants early in adult life .* **Journal of Insect Science, 11, art. no. 67, pp.1-9**

ABSTRACT: Although multiple lines of evidence suggest that early adult life is very important in shaping the reproductive behavior of males, few studies have looked at the fitness consequences of the variation in reproductive behavior induced by differences in early life experience of males. Using a long term laboratory adapted population of Drosophila melanogaster Meigen (Diptera: Drosophilidae), early life experience, in terms of co-inhabitant numbers, was found to affect male mating behavior and at least one fitness component. However, in contrast to previous studies, a non-linear relationship was found between early life experience and fitness components and a significant effect of co-inhabitant number on copulation duration and sperm defense. Both these traits showed a sharp increase as the co-inhabitant numbers changed from 1 to 16. However, there was a decline in the trait values as the co-inhabitant number increased further. The probable causes for the observed non-linear pattern of responses are discussed.

KEYWORDS: Diptera; Drosophila melanogaster; Drosophilidae, animal; article; copulation; Drosophila melanogaster; female; male; physiology; spermatozoon, Animals; Copulation; Drosophila melanogaster; Female; Male; Spermatozoa

http://www.bioone.org/doi/abs/10.1673/031.011.6701?url_ver=Z39.88-2003&rfr_id=ori:rid:crossref.org&rfr_dat=cr_pub%3dpubmed&

doi: http://dx.doi.org/10.1673/031.011.6701

119. Matsyendranath Shukla., Kavita Dorai (2011) *Resolving overlaps in diffusion encoded spectra using band-selective pulses in a 3D BEST-DOSY experiment* . **Journal of Magnetic Resonance, 213 (1), pp. 69-75**.

ABSTRACT: A novel diffusion-edited 3D NMR experiment that incorporates a BEST-HMQC pulse sequence in its implementation is presented. Heteronuclear 3D DOSY NMR experiments are useful in elucidating the diffusion coefficients of individual constituents of a mixture, especially in cases where the proton NMR 2D DOSY spectra show considerable overlap. The present 3D BEST-DOSY pulse sequence provides a more sensitive and less time-consuming alternative to standard 3D HMQC-DOSY experiments. Cleanly separated subspectra of individual mixture components are obtained, leading to the determination of diffusion coefficients with better accuracy. The feasibility of the technique is demonstrated on a mixture of amino acids, on a mixture of small molecules with similar diffusion coefficients, and on a complex mixture with large dynamic range (commercial gasoline). The implications of using adiabatic decoupling schemes and band-selective shaped pulses for selective BEST-DOSY experiments on proteins are also discussed. © 2011 Elsevier Inc. All rights reserved.

KEYWORDS: BEST-HMQC; Carbon-13; Diffusion ordered spectroscopy (DOSY); Heteronuclear; Pulsed field gradients, Amino acids; Experiments; Mixtures; Nuclear magnetic resonance spectroscopy; Three dimensional, Diffusion, amino acid; camphene; carbon; deuterium oxide; gasoline; geraniol; lysozyme; protein; quinine; terpene; water, algorithm; article; chemical model; chemistry; diffusion; electromagnetic field; methodology; nuclear magnetic resonance; reproducibility; signal noise ratio, Algorithms; Amino Acids; Carbon Isotopes; Deuterium Oxide; Diffusion; Electromagnetic Fields; Gasoline; Models, Chemical; Muramidase; Nuclear Magnetic Resonance, Biomolecular; Proteins; Quinine; Reproducibility of Results; Signal-To-Noise Ratio; Terpenes; Water

http://www.sciencedirect.com/science/article/pii/S1090780711003089

http://dx.doi.org/10.1016/j.jmr.2011.08.038

120. Gurmeet K Bakshi., **Shalini Gupta., Inder Bir S Passi (2011)** *Semisimple metacyclic group algebras* **Proceedings of the Indian Academy of Sciences: Mathematical Sciences, 121 (4), pp. 379-396.**

ABSTRACT: Given a group G of order p1 p2, where p1, p2 are primes, and Fq, a finite field of order q coprime to p1 p2, the object of this paper is to compute a complete set of primitive central idempotents of the semisimple group algebra Fq [G]. © Indian Academy of Sciences.

KEYWORDS: Automorphism groups; Coprime; Finite fields; Idempotents, Binary sequences, Algebra

www.ias.ac.in/mathsci/vol121/nov2011/pmsc-d-10-00210.pdf

121. K. Imroze., **N. G. Prasad (2011)** *Sex-specific effect of bacterial infection on components of adult fitness in Drosophila melanogaster.* **Journal of Evolutionary Biology Research, 3: 79-86 (2011).**

ABSTRACT: We investigated the sex specific effect of Serratia marcescens infection through septic injury on two components of fitness, survivorship and adult competitive reproductive fitness in male and female Drosophila melanogaster. Under competitive conditions, infected females showed significantly lower reproductive output compared to control females. However, male reproductive fitness was not affected by infection. We did not find any cost of injury and immune deployment in our study indicating that the fitness cost resulted only from sustained infection or virulence. However, the bacteria was found to be pathogenic, growing equally well in males and females and causing about 80% mortality over an eleven day period with no significant difference in mortality between sexes. Thus, such sex specific effects of pathogens on individual components of fitness indicate that the total fitness cost experienced by each sex might be very different, even within a given regime, thereby affecting the evolution of antibacterial immunity.

KEYWORDS: Sex-specific effect, fitness, survivorship, Serratia marcescens, Drosophila melanogaster

http://www.academicjournals.org/JEBR

www.researchgate.net/...Sex-specific_effect_of_bacterial_infection_o...

122. Rajesh Kochhar (2011) _Smallpox in the modern scientific and colonial contexts 1721-1840_. **Journal of biosciences, 36 (5), pp. 761-768.**

KEYWORDS: article; cowpox; Cowpox virus; history; human; immunology; smallpox; vaccination, Cowpox; Cowpox virus; History, 17th Century; History, 18th Century; History, 19th Century; Humans; Smallpox; Vaccination

http://link.springer.com/article/10.1007%2Fs12038-011-9146-6?LI=true#page-1

DOI 10.1007/s12038-011-9146-6

123. Ville Keranen., Esko Keski-Vakkuri., Sean Nowling., **K. P. Yogendran (2011)** _Solitons as Probes of the Structure of Holographic Superfluids,_ **New J. Phys. 13, 065003 .**

ABSTRACT : The detailed features of solitons in holographic superfluids are discussed. Using solitons as probes, we study the behavior of holographic superfluids by varying the scaling dimension of the condensing operator and make a comparison to the Bose–Einstein condensate–Bardeen–Cooper–Schrieffer comparison phenomena. Further evidence of this analogy is provided by the behavior of the solitons' length scales as well as by the superfluid critical velocity.

KEYWORDS: Quantum gases, liquids and solids ;Particle physics and field theory ;Statistical physics and nonlinear systems

http://iopscience.iop.org/1367-2630/13/6/065003

doi:10.1088/1367-2630/13/6/065003

124. Roman Mikhailov., **Inder Bir S. Passi.**, Jie Wu **(2011)** _Symmetric ideals in group rings and simplicial homotopy_ . **Journal of Pure and Applied Algebra, 215 (5), pp. 1085-1092.**

ABSTRACT: In this paper homotopical methods for the description of subgroups determined by ideals in group rings are introduced. It is shown that in certain cases the subgroups determined by symmetric product of ideals in group rings can be described with the help of homotopy groups of spheres. © 2010 Elsevier B.V.

http://repository.ias.ac.in/56788/

http://www.sciencedirect.com/science/article/pii/S0022404910001672

http://dx.doi.org/10.1016/j.jpaa.2010.07.013

125. Hiroyasu Ando., **Sudeshna Sinha.**, Remo Storni., Kazuyuki Aihara **(2011)** *Synthetic gene networks as potential flexible parallel logic gates* . ***EPL, 93 (5), art. no. 50001, .***

ABSTRACT: We show how a synthetic gene network can function, in an optimal window of noise, as a robust logic gate. Interestingly, noise enhances the reliability of the logic operation. Further, the noise level can also be used to switch logic functionality, for instance toggle between AND, OR and XOR gates. We also consider a two-dimensional model of a gene network, where we show how two complementary gate operations can be achieved simultaneously. This indicates the flexible parallel processing potential of this biological system. © 2011 Europhysics Letters Association

http://iopscience.iop.org/0295-5075/93/5/50001

doi:10.1209/0295-5075/93/50001

126. Pratibha Kapoor., Ajay Pal Singh Pannu., Mukesh Sharma., Geeta Hundal., **Ramesh Kapoor.**, Maninder Singh Hundal **(2011)** *Syntheses and structures of cobalt(II), nickel(II), and copper(II) complexes with N,N,N′,N′-tetraalkylpyridine-2,6-dicarboxamides (O-daap) containing nitrate as the counter ion.* **Journal of Coordination Chemistry, 64 (2), pp. 256-271.**

ABSTRACT: Reactions of M(NO_3)$_2$ xH_2O [M = Co(II), Ni(II), and Cu(II)] with N,N,N',N'-tetraalkylpyridine-2,6-dicarboxamides(O-daap) in CH_3CN yield [Co(O-dmap)(NO_3)$_2$] (1), [Co(O-deap)(NO_3)$_2$] (2), [Co(O-dpap)(NO_3)$_2$] (3), [Ni(O-dmap)(H_2O)$_3$](NO_3)$_2$ (4), [Ni(O-deap)(H_2O)$_2$(NO_3)](NO_3)] (5), [Cu(O-deap)(NO_3)$_2$] (6), and [Cu(O-dpap)(NO_3)$_2$](7). X-ray crystal structures of 1, 2, 4, 5, and 7 reveal that O-daap ligands coordinate tridentate to each metal, O-N-O, with nitrate playing a vital role in molecular and crystal structures of all the complexes. The coordination geometry in the two Co(II) complexes, 1 and 2, is approximately pentagonal bipyramidal with nitrate bonded in a slightly unsymmetrical bidentate chelating mode. $[Ni(dmap)(H_2O)_3](NO_3)_2$ (4) and $[Ni(deap)(H_2O)_2(NO_3)]$ (NO_3) (5) exhibit octahedral geometry, the former containing uncoordinated nitrate while the latter has one nitrate coordinated unidentate and the other nitrate outside the coordination sphere. The Cu(II) in [Cu(dpap)(NO$_{3)2}$] (7) occupies a distorted square pyramidal geometry and is linked to two unidentate nitrates, although one nitrate is also involved in a weak interaction with the metal through its other oxygen. IR spectra and other physical studies are consistent with their crystal structural data. O-dmap = N,N,N',N'-tetramethylpyridine-2,6-dicarboxamides; O-deap = N,N,N',N'-tetraethylpyridine-2,6-dicarboxamides; and O-dpap = N,N,N',N'-tetraisopropylpyridine-2,6-dicarboxamides. © 2011 Taylor & Francis.

KEYWORDS: Counterion; Crystal structure; Square pyramidal; Thermogravimetric

http://dx.doi.org/10.1080/00958972.2010.542237

http://www.tandfonline.com/doi/abs/10.1080/00958972.2010.542237

DOI:10.1080/00958972.2010.542237

127. M. Brydon-Miller., M. Kral, P. Maguire., S. Noffke., **A. Sabhlok** Jazz **(2011)** *the Banyan tree: Roots and Riffs in Participatory Action Research.* In : **Denzin, N (ed.) Handbook of Qualitative Research, p.387-400. Sage publications.**

http://www.sagepub.com/books/Book233401#tabview=toc

128. Melina Grigorian., **Lolitika Mandal.**, Manuel Hakimi., Irma Ortiz., Volker Hartenstein **(2011)** *The convergence of Notch and MAPK signaling specifies the blood progenitor fate in the Drosophila mesoderm.* **Developmental Biology, 353 (1), pp. 105-118.**

ABSTRACT: Blood progenitors arise from a pool of pluripotential cells ("hemangioblasts") within the Drosophila embryonic mesoderm. The fact that the cardiogenic mesoderm consists of only a small number of highly stereotypically patterned cells that can be queried individually regarding their gene expression in normal and mutant embryos is one of the significant advantages that Drosophila offers to dissect the mechanism specifying the fate of these cells. We show in this paper that the expression of the Notch ligand Delta (Dl) reveals segmentally reiterated mesodermal clusters ("cardiogenic clusters") that constitute the cardiogenic mesoderm. These clusters give rise to cardioblasts, blood progenitors and nephrocytes. Cardioblasts emerging from the cardiogenic clusters accumulate high levels of Dl, which is required to prevent more cells from adopting the cardioblast fate. In embryos lacking Dl function, all cells of the cardiogenic clusters become cardioblasts, and blood progenitors are lacking. Concomitant activation of the Mitogen Activated Protein Kinase (MAPK) pathway by Epidermal Growth Factor Receptor (EGFR) and Fibroblast Growth Factor Receptor (FGFR) is required for the specification and maintenance of the cardiogenic mesoderm; in addition, the spatially restricted localization of some of the FGFR ligands may be instrumental in controlling the spatial restriction of the Dl ligand to presumptive cardioblasts. © 2011 Elsevier Inc.

KEYWORDS: epidermal growth factor receptor; mitogen activated protein kinase; Notch receptor, animal cell; animal tissue; article; cardioblast; cell count; cell fate; controlled study; Drosophila; embryo; embryo development; enzyme activation; gene expression; hemangioblast; hematopoietic stem cell; mesoderm; nephrocyte; nonhuman; pluripotent stem cell; priority journal; protein expression; protein localization; signal transduction; stem cell, Animals; Basic Helix-Loop-Helix Transcription Factors; Body Patterning; DNA-Binding Proteins; Drosophila melanogaster; Drosophila Proteins; Epidermal Growth Factor; Fibroblast Growth Factors; Hematopoietic Stem Cells; MAP Kinase Signaling System; Mesoderm; Morphogenesis; Receptors, Notch

www.sciencedirect.com/science/article/pii/S0012160611001400

http://dx.doi.org/10.1016/j.ydbio.2011.02.024

129. Pradeep Kumar., **N.Sathyamurthy (2011)** T*heoretical studies of host - Guest interaction in gas hydrates* . **Journal of Physical Chemistry A, 115 (50), pp. 14276-14281**.

ABSTRACT: Ab initio calculations and atoms-in-molecules (AIM) analysis have been used to investigate the host - guest interaction in dodecahedral water cages using a variety of guest species that include monatomic (He, Ne, Ar, Kr, and Xe), diatomic (CO, H_2, N_2, O_2, and NO), triatomic (CO_2, NO_2, and O_3) and polyatomic (CH_4 and NH_3) molecules. Geometry optimization for the guest species, host cage, and their complexes was carried out using the second order Müller - Plesset perturbation method with the 6-31G ** basis set. Single point energy calculations using the same method but different basis sets (6-31++G **, 6-311++G **, aug-cc-pVDZ, and aug-cc-pVTZ) were carried out for the MP2/6-31G ** optimized geometries. The interaction energy between the guest species and the host cage has been obtained in the complete basis set limit by basis set extrapolation. (Figure presented) © 2011 American Chemical Society.

KEYWORDS: Ab initio calculations; Atoms-in-molecules; Basis sets; Complete basis set limit; Geometry optimization; Guest species; Interaction energies; MP2/6-31G; Optimized geometries; Perturbation method; Polyatomics; Second orders; Single-point energy; Theoretical study; Water cage, Calculations; Carbon dioxide; Krypton; Neon; Optimization; Perturbation techniques; Xenon, Gas hydrates

http://pubs.acs.org/doi/abs/10.1021/jp2089565

DOI: 10.1021/jp2089565

130. Neal S. Gupta (2011) *Transformation of chitinous tissues in elevated P-T conditions: additional insights from experiments from plant tissues*, **Topics in Geobiology 34 : pp.,153-168**

ABSTRACT : Modern arthropod cuticles consist of chitin protein complex, but fossil arthropods older than Cenozoic, contain a significant amount of aliphatic component with or without any chitin. Such a transformation is observed in leaves of plant fossils where the bulk composition has been modified. This

apparent contradiction was examined by subjecting modern animal cuticles to confined heating (350°C/700 bars/24 h) following various chemical treatments. Analysis of artificially matured untreated cuticle, yielded moieties related to phenols and alkylated substituents, pyridines, pyrroles and possibly indenes (from chitin). Components such as *n*-alkyl amides, fatty acids and alkane/alkene homologues ranging from C9 to <C20 were also generated, indicating the presence of an *n*-alkyl component, similar in composition to that encountered in fossil arthropods. Analysis of cuticles that had been heated after lipid extraction and hydrolysis did not yield any aliphatic polymer. This provides evidence that lipids incorporated from the cuticle were the source of aliphatic polymer. Similar heating of plant tissues generated an aliphatic macromolecule similar to that found in fossils. Comparison of the products derived from maturation of differentpre-treated plant tissues demonstrates that solvent-extractable and hydrolysable lipids were precursors of the generated macromolecular material. Thus, the experiments indicate that labile alkyl compounds can be a source of the insoluble aliphatic component of fossil organic matter in the absence of a resistant aliphatic precursor in the living organism.

http://link.springer.com/chapter/10.1007/978-90-481-9684-5_8

DOI:10.1007/978-90-481.9684-5_8

131. Karan Paul., Kausik Chattopadhyay (2011) *Unfolding distinguishes the Vibrio cholerae cytolysin precursor from the mature form of the toxin* .**Biochemistry, 50 (19), pp. 3936-3945.**

ABSTRACT: Vibrio cholerae cytolysin (VCC) is a potent cytolytic toxin that induces colloid osmotic lysis of its target eukaryotic cells by forming transmembrane oligomeric β-barrel channels. VCC is secreted by the bacteria as an inactive precursor (Pro-VCC) and is subsequently activated by proteolytic removal of an N-terminal "Pro-domain", thus generating the active form of the toxin (Mature-VCC). Earlier studies have indicated an intramolecular chaperone-like role of the Pro-domain favoring efficient secretion of the toxin from the periplasm into the extracellular space. However, the exact role of the Pro-domain in the VCC structure-function mechanism remains unclear. Here, we have

compared the Pro-VCC and Mature-VCC molecules in terms of their structural and conformational properties. We have studied unfolding of the two variants of the VCC molecule in response to an array of denaturing conditions, including low-pH, chemical denaturant and heat-induced unfolding. Pro-VCC shows a more profound tendency to unfold in response to such denaturing conditions compared to Mature-VCC. Biophysical characterization of the isolated Pro-domain further suggests that the increased unfolding propensity of Pro-VCC does not arise because of an increased level of unfolding of the Pro-region itself. Altogether, our results imply that a natively folded architecture of the Pro-VCC molecule with sufficient structural and conformational plasticity presumably allows it to adopt a suitable configuration that is possibly required for its efficient secretion and subsequent proteolytic maturation under physiological conditions. © 2011 American Chemical Society.

KEYWORDS: Biophysical characterization; Chemical denaturants; Colloid-osmotic lysis; Conformational plasticity; Conformational properties; Cytolytic toxin; Denaturing conditions; Eukaryotic cells; Extracellular space; N-terminals; Periplasm; Physiological condition; Transmembranes; Vibrio cholerae, Conformations; Molecules; Oligomers; Physiology, Toxic materials, cholera toxin; cytolysin; tryptophan, article; denaturation; fluorescence; pH; priority journal; protein binding; protein conformation; protein folding; protein structure; Vibrio cholerae, Bacterial Outer Membrane Proteins; Cholera Toxin; Cytotoxins; Enzyme Precursors; Hydrogen-Ion Concentration; Pore Forming Cytotoxic Proteins; Protein Structure, Tertiary; Protein Transport; Protein Unfolding; Vibrio cholerae, Eukaryota; Vibrio cholerae

http://pubs.acs.org/doi/abs/10.1021/bi200332g

DOI: 10.1021/bi200332g

132. Vadla Rajkumar., Nayyar Ahmad Aslam., Chennakesava Reddy., Srinivasarao Arulananda Babu (2011) *Unactivated Norbornenes in [3+2] Cycloadditions: Remarkably Stereocon- trolled Entry into Norbornane-Fused-Spirooxindolopyrrolidines, Spiro-1,3- in- dandionolylpyrrolidines and Spirooxindolopyrrolizidines,* **Synlett, 23, 549-556**

ABSTRACT :1,3-dipolar cycloaddition reactions of azomethine ylides with unactivated norbornene dipolarophiles and a highly diastereoselective synthesis of the novel norbornane-fused spirooxindolopyrrolidines, spiroacenaphthylenolylpyrrolidines, spiro-1,3-indandionolylpyrrolidines, and spirooxindolopyrrolizidines having an array of stereocenters are reported. The stereoselective synthesis of spirooxindolopyrrolizidines with eight stereocenters was demonstrated. Single-crystal X-ray structural analyses were performed to unambiguously establish the structure and stereochemistry of the key products.

KEYWORDS : 1,3-dipolar cycloaddition, oxindoles, spiro compounds, stereoselective synthesis, ylides

https://www.thieme-connect.de/ejournals/pdf/10.1055/s-0031-1290342.pdf

DOI: 10.1055/s-0031-1290342; Art ID: D52011ST

133. G.S.S.Saini., Sarvpreet Kaur., S.K.Tripathi., Sukh Dev Dogra., Jasim M. Abbas., **C.G.Mahajan (2011)***Vibrational spectroscopic and density functional theory studies of chloranil-imidazole interaction.* **Vibrational Spectroscopy, 56 (1), pp. 66-73.**

ABSTRACT: The present work reports vibrational spectra and density functional theory calculations for chloranil, imidazole and their complexes. The experimentally observed infrared and Raman bands have been assigned with the help of calculated vibrational frequencies and potential energy distribution analysis. Some bands of chloranil and imidazole have been found to shift on the complex formation due to partial electronic charge transfer from imidazole to chloranil. The charge transfer between these molecules is also corroborated by the electronic absorption spectroscopy and calculations. The theoretical values of the interaction energy of various possible chloranil-imidazole interactions suggest that the two molecules interact preferably via N and H atoms of imidazole and CO group of chloranil with their molecular planes almost perpendicular to each other. © 2010 Elsevier B.V. All rights reserved.

KEYWORDS: Chloranil; Density functional theory calculations; Imidazole; Infrared spectrum; Raman spectra; UV-vis spectra, Absorption spectroscopy; Charge transfer; Complexation; Ion exchange; Mass transfer; Raman scattering; Raman spectroscopy, Density functional theory

http://www.sciencedirect.com/science/article/pii/S092420311000158X

http://dx.doi.org/10.1016/j.vibspec.2010.10.004,

Titles
A - Z : 2012

2012

134. Krishnendu Gongopadhyay (2012) *Algebraic Characterization of isometries of the hyperbolic 4-space*, **ISRN Geometry 2012, Article ID 757489.**

ABSTRACT: We classify isometries of the real hyperbolic \$4\$-space by their conjugacy classes of centralizers. We use the representation of the isometries by 2x2 quaternionic matrices to obtain this characterization. Another characterization in terms of conjugacy invariants is also obtained as an appendix to our earlier work

KEYWORDS : hyperbolic 4-space, classification of isometries, quaternions.

http://www.isrn.com/journals/geometry/2012/757489/

doi:10.5402/2012/757489

135. Ashok Ajoy., Rama Koteswara Rao., Anil Kumar., **Pranaw Rungta (2012)** *Algorithmic approach to simulate Hamiltonian dynamics and an NMR simulation of quantum state transfer.* **Physical Review A - Atomic, Molecular, and Optical Physics, 85 (3), art. no. 030303, .**

ABSTRACT: We propose an iterative algorithm to simulate the dynamics generated by any n-qubit Hamiltonian. The simulation entails decomposing the unitary time evolution operator U (unitary) into a product of different time-step unitaries. The algorithm product-decomposes U in a chosen operator basis by identifying a certain symmetry of U that is intimately related to the number of gates in the decomposition. We illustrate the algorithm by first obtaining a polynomial decomposition in the Pauli basis of the n-qubit quantum state transfer unitary by Di Franco that transports quantum information from one end of a spin chain to the other, and then implement it in nuclear magnetic resonance to demonstrate that the decomposition is experimentally viable. We further experimentally test the resilience of the state transfer to static errors in the coupling parameters of the simulated Hamiltonian. This is done by decomposing and simulating the corresponding imperfect unitaries. © 2012 American Physical Society.

KEYWORDS: Algorithmic approach; Coupling parameters; Hamiltonian dynamics; Iterative algorithm; Number of gates; Quantum Information; Quantum state transfers; Spin chains; State transfer; Static error; Time evolution operator; Time step, Algorithms; Dynamics; Hamiltonians; Quantum computers; Quantum theory, Quantum optics

http://pra.aps.org/abstract/PRA/v85/i3/e030303

DOI:10.1103/PhysRevA.85.030303

136. Wensheng Cao., **Krishnendu Gongopadhyay (2012)** *Algebraic characterization of isometries of the complex and the quaternionic hyperbolic planes* . **Geometriae Dedicata, 157 (1), pp. 23-39.**

ABSTRACT: Let H F 2 denote the two dimensional hyperbolic space over F, where F is either the complex numbers ℂ or the quaternions ℍ. It is of interest to characterize algebraically the dynamical types of isometries of H F 2. For F = ℂ, such a characterization is known from the work of Giraud-Goldman. In this paper, we offer an algebraic characterization of isometries of H ℍ 2. Our result restricts to the case F = ℂ and provides another characterization of the isometries of H ℂ 2, which is different from the characterization due to Giraud-Goldman. Two elements in a group G are said to be in the same z-class if their centralizers are conjugate in G. The z-classes provide a finite partition of the isometry group. In this paper, we describe the centralizers of isometries of H F 2 and determine the z-classes. © 2011 Springer Science+Business Media B.V.

KEYWORDS: Classification of isometries; Complex and quaternionic hyperbolic space; z-class

http://link.springer.com/article/10.1007%2Fs10711-011-9599-7?LI=true

DOI 10.1007/s10711-011-9599-7

137. S.Srivastava., **N.Sathyamurthy.,** A.J.C.Varandas (**2012**) *An accurate ab initio potential energy curve and the vibrational bound states of* $X^2\ \Sigma u^+$ *state of* H_2^- **Chemical Physics, 398 (1), pp. 160-167.**

ABSTRACT: Potential energy curve for the $X_2\Sigma u^+$ state of H_2^- has been computed at the full CI/cc-pVXZ (X = D - Q) level. An analytic function is fitted to the resulting potential energy curve and is then used to calculate the vibrational bound states of H_2^- and compared with those for H_2. © 2011 Elsevier B.V. All rights reserved.

KEYWORDS: Anions; Electron scattering; H_2^-., Potential energy curve

http://www.sciencedirect.com/science/article/pii/S0301010411003910

http://dx.doi.org/10.1016/j.chemphys.2011.08.023,

138. . **Freeda D’cruz, Adrene (2012)** *An Inconvenient Truth: The Quandary of Dystopian Earth in Douglas Trumbull’s Silent Running and Richard Fleischer’s Soylent Green*. **The IUP Journal of American Literature, 5(1) pp. 7-15,**

ABSTRACT: Ecocide, the widespread annihilation of nature, constitutes the principal theme of Douglas Trumbull’s Silent Running (1972) and Richard Fleischer’s Soylent Green (1973). Seeking recourse to one of the major film genres, namely, science fiction, these films emphatically disclose an inconvenient truth - the imminent extinction of the ecosystem. Set in a dystopian world, the films outline two futuristic probabilities: the sustenance of the last trace of bio-network only on spaceships in Silent Running and the overpopulated city haunted by the scarcity of natural resources in Soylent Green. In other words, while Silent Running strategically uncovers an already depleted biosphere, Soylent Green systematically examines the road to ecological perdition. Significantly, the cinematic space resorts to diverse techniques, including stills, close-up, voice-over, and music, to convey the petrifying reality that awaits humanity in the near future. Drawing the title from Davis Guggenheim’s An Inconvenient Truth, a documentary on global warming, this paper, in analyzing the environmental apocalypse in Silent Running and Soylent Green, seeks to reveal how the cinematography weaves an ecocentric discourse to promote the inevitable truth that ecosphere is intrinsic to human survival.

KEYWORDS: Ecocide, Bio-network, Ecosphere, An Inconvenient Truth, Cinematography, and Ecological perdition.
http://connection.ebscohost.com/c/articles/78153732/inconvenient-truth-quandary-dystopian-earth-douglas-trumbulls-silent-running-richard-fleischers-soylent

139. Samrat Ghosh., Shilpa Setia., Sumyra Sidiq., Santanu Kumar Pal (2012) *A new visual test for p-quinone and its relevance to the biodiesel industry*. **Analytical Methods, 4 (11), pp. 3542-3544.**

ABSTRACT: The production of biodiesel fuel (BDF) from vegetable oil using a co-solvent such as acetone has been demonstrated to be a green technique for large scale production of BDF under ambient conditions. However, it is the acetone removal step which involves input of energy and, therefore, any optimization of the acetone recovery process in terms of heating duration will make it more cost effective. The presence of acetone in the BDF synthesized according to the above technique can be routinely monitored using laborious spectroscopic techniques. However, colour specific tests will prove to be quick, convenient, less expensive and can be performed by an individual on the production site as frequently as required. Herein we report a new colour test for the detection of acetone which can also be applied to the detection of tert-butyl hydroquinone (TBHQ), a well-known antioxidant in vegetable oil and BDF. © 2012 The Royal Society of Chemistry.

KEYWORDS: Ambient conditions; Bio-diesel fuel; Biodiesel industry; Cosolvents; Cost effective; Green techniques; Large scale productions; Production sites; Recovery process; Spectroscopic technique, Biodiesel; Phenols; Vegetable oils, Acetone

http://pubs.rsc.org/en/content/articlehtml/2012/ay/c2ay25591j?page=search

DOI: 10.1039/C2AY25591J

140. Matsyendranath Shukla., Kavita Dorai (2012) *A Novel Multiple-Quantum Correlation NMR Scheme to Separate Components of a Mixture According to Their Diffusion Coefficients*. Applied Magnetic Resonance, 43 (4), pp. 485-497.

ABSTRACT: A versatile three-dimensional diffusion-edited nuclear magnetic resonance experiment is described that concatenates a multiple-quantum/single-quantum correlation scheme with a diffusion-ordered pulse sequence. The experiment is demonstrated on mixtures of small molecules with similar diffusion coefficients and is able to resolve severely overlapped signals along the

third dimension. The subspectra of individual components of the mixtures are well separated and their diffusion coefficients can hence be extracted with a greater degree of accuracy as compared to the standard two-dimensional diffusion-ordered spectroscopy experiments. © 2012 Springer-Verlag.

KEYWORDS: Correlation scheme; Degree of accuracy; Individual components; Pulse sequence; Small molecules, Experiments; Mixtures; Separation, Diffusion

link.springer.com/article/10.1007/s00723-012-0316-y/fulltext.html

DOI: 10.1007/s00723-012-0316-y

141. Moumita Majumder., **N. Sathyamurthy (2012)** *A Theoretical Investigation on the Effect of $\pi - \pi$ stacking Interaction on ^{1} H Isotropic Chemical Shielding in Certain Homo- and Hetero- nuclear Aromatic Systems, Theoretical Chemistry Accounts*: **Theoretical Chemistry Accounts:Theory, Computation, and Modeling (Theoretica Chimica Acta) 131, PP.1092**

ABSTRACT : Significant changes in the proton chemical shielding (and hence the chemical shift) are predicted in going from the monomer to the dimer of benzene, naph- thalene, pyridine and quinoline systems and also the trimer of benzene and pyridine. The computed NMR spectra show additional splitting in going from the monomer to the dimer and the trimer of different species. The aromatic protons show a significant upfield shift due to the enhancement of anisotropic shielding by the p electron cloud of the neighboring molecule(s). The nature of the NMR spectra also changes with the orientation of the stacked conform- ers. The results obtained using Møller-Plesset second-order perturbation theory along with the GIAO method show the changes in isotropic shielding, in a reasonable basis set independent fashion. © 2012 Springer-Verlag.

KEYWORDS : p–p Stacking Á NMR Á Aromatic systems Á ;Proton chemical shielding

http://link.springer.com/article/10.1007%2Fs00214-012-1092-3

DOI 10.1007/s00214-012-1092-3

142. Christopher Pöhlker., Kenia T. Wiedemann., **Bärbel Sinha.**, Manabu Shiraiwa., Sachin S. Gunthe., Mackenzie Smith., Hang Su., Paulo Artaxo., Qi Chen., Yafang Cheng., Wolfgang Elbert., Mary K. Gilles., Arthur L. D. Kilcoyne., Ryan C. Moffet., Markus Weigand., Scot T. Martin., Ulrich Pöschl., Meinrat O. Andreae(**2012**) *Biogenic potassium salt particles as seeds for secondary organic aerosol in the Amazon.* **Science, 337 (6098), pp. 1075-1078.**

ABSTRACT: The fine particles serving as cloud condensation nuclei in pristine Amazonian rainforest air consist mostly of secondary organic aerosol. Their origin is enigmatic, however, because new particle formation in the atmosphere is not observed. Here, we show that the growth of organic aerosol particles can be initiated by potassium-salt - rich particles emitted by biota in the rainforest. These particles act as seeds for the condensation of low- or semi-volatile organic compounds from the atmospheric gas phase or multiphase oxidation of isoprene and terpenes. Our findings suggest that the primary emission of biogenic salt particles directly influences the number concentration of cloud condensation nuclei and affects the microphysics of cloud formation and precipitation over the rainforest.

KEYWORDS: isoprene; potassium salt; terpene; volatile organic compound, aerosol; atmospheric gas; cloud condensation nucleus; oxidation; potassium; pristine environment; rainforest; salt; volatile organic compound, article; biota; cloud; oxidation; particle size; precipitation; priority journal; rain forest; scanning electron microscopy; scanning transmission electron microscopy; secondary organic aerosol; X ray absorption spectroscopy, Atmosphere; Particle Size; Particulate Matter; Potassium; Rain; Salts; South America; Trees, Amazon River

http://www.sciencemag.org/content/337/6098/1075.full

DOI: 10.1126/science.1223264

143. B.J.H.Van Stratum., J.Vilá-Guerau De Arellano., H.G.Ouwersloot, K.Van Den Dries., T.W.Van Laar., M.Martinez., J.Lelieveld., J.-M.Diesch, F.Drewnick., H.Fischer., Z.Hosaynali Beygi., H.Harder., E.Regelin., **V. Sinha,** J.A.Adame., M.Sörgel., R.Sander., H.Bozem., W.Song., J.Williams., N.Yassaa (**2012**) *Case study of the diurnal variability of chemically active species with respect to boundary layer dynamics during DOMINO*. **Atmospheric Chemistry and Physics, 12 (12), pp. 5329-5341.**

ABSTRACT: We study the interactions between atmospheric boundary layer (ABL) dynamics and atmospheric chemistry using a mixed-layer model coupled to chemical reaction schemes. Guided by both atmospheric and chemical measurements obtained during the DOMINO (Diel Oxidant Mechanisms in relation to Nitrogen Oxides) campaign (2008), numerical experiments are performed to study the role of ABL dynamics and the accuracy of chemical schemes with different complexity: the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4) and a reduced mechanism of this chemical system. Both schemes produce satisfactory results, indicating that the reduced scheme is capable of reproducing the O 3-NO x-VOC-HO x diurnal cycle during conditions characterized by a low NO x regime and small O 3 tendencies (less than 1 ppb per hour). By focusing on the budget equations of chemical species in the mixed-layer model, we show that for species like O 3, NO and NO 2, the influence of entrainment and boundary layer growth is of the same order as chemical production/loss. This indicates that an accurate representation of ABL processes is crucial in understanding the diel cycle of chemical species. By comparing the time scales of chemical reactive species with the mixing time scale of turbulence, we propose a classification based on the DamkÃ¶hler number to further determine the importance of dynamics on chemistry during field campaigns. Our findings advocate an integrated approach, simultaneously solving the ABL dynamics and chemical reactions, in order to obtain a better understanding of chemical pathways and processes and the interpretation of the results obtained during measurement campaigns. © 2012 Author(s).

KEYWORDS: atmospheric chemistry; boundary layer; chemical reaction; diurnal variation; mixed layer; numerical model; ozone; turbulence

www.atmos-chem-phys.net/12/5329/2012/

doi:10.5194/acp-12-5329-2012

144. Sujitha Kolakkandy., Kousik Giri., **N. Sathyamurthy** **(2012)** *Collision-induced dissociation in (He, H_2^+ (v = 0-2; J = 0-3)) system: A time-dependent quantum mechanical investigation .* **Journal of Chemical Physics, 136 (24), art. no. 244312, .**

ABSTRACT: The collision-induced process He + H_2^+ (v=0-2;j=0-3)→ He +H+H + has been investigated using a time-dependent quantum mechanical wave packet approach, within the centrifugal sudden approximation. The exchange reaction He + H_2^+ → HeH^+ + H, which has a lower threshold, dominates over the dissociation process over the entire energy range considered in this study. The reaction cross section for both the exchange and dissociation channels and the branching ratio between the two channels have been computed on the McLaughlin-Thompson- Joseph-Sathyamurthy potential-energy surface and compared with the available experimental and quasiclassical trajectory results. © 2012 American Institute of Physics.

KEYWORDS: Branching ratio; Centrifugal sudden; Collision-induced dissociation; Dissociation channels; Dissociation process; Energy ranges; Exchange reaction; Quantum mechanical; Quasiclassical trajectories; Reaction cross-sections; Time-dependent; Two channel, Centrifugation; Quantum theory, Dissociation

http://jcp.aip.org/resource/1/jcpsa6/v136/i24/p244312_s1?isAuthorized=no

http://scitation.aip.org/getpdf/servlet/GetPDFServlet?filetype=pdf&id=JCPSA6000136000024244312000001&idtype=cvips&doi=10.1063/1.4729255&prog=normal

http://dx.doi.org/10.1063/1.4729255

145. Pushpender K Sharma., Vinodh Kumar., Jagdeep Kaur **(2012)** *Common Methods Employed in Directed Evolution and Their Application in Modification of Lipases.* **Research Journal of Pharmaceutical, Biological and Chemical Sciences, 3 (3), pp. 183-191.**

ABSTRACT Biocatalyst plays an important role in the catalysis of biochemical/chemical reactions. Unfortunately, the majority of natural occurring enzyme lacks characteristic features essentially required during industrial processes e.g. thermostability/solvent stability/enantio-selectivity. Protein engineering methods play an important role in altering the natural properties of the enzymes i.e. protein thermostability, catalytic efficiency, tolerance towards

extreme pH, activity and stability in presence of organic solvents. Directed evolution has emerged as useful technique that can produce variants, prior the knowledge of three dimensional structures. This review article discusses most common methods that are employed in modification of industrially relevant enzymes. Since, past several years so our lab is working in lipases, therefore we are discussing the application of directed evolution in altering the function of lipases.

KEYWORDS: Biocatalyst, directed evolution, error prone PCR, enantio-selectivity

http://www.researchgate.net/publication/235327359_Common_Methods_Employed_in_Directed_Evolution_and_Their_Application_in_Modification_of_Lipase

146. Subrahmanya Ishwar Bhat., **Angshuman Roy Choudhury.**, Darshak R. Trivedi (**2012**) *Condensation of malononitrile with salicylaldehydes and o-aminobenzaldehydes revisited: Solvent and catalyst free synthesis of 4H-chromenes and quinoline*s. **RSC Advances, 2 (28), pp. 10556-10563.**

ABSTRACT: The reaction of malononitrile with salicylaldehyde under solvent and catalyst free conditions was re-investigated using mechanochemical mixing, thermal heating and a direct crystallization process. The resulting condensation product by all three types of molecular activation, was found to be (2-amino-3-cyano-4H-chromene-4-yl)malononitrile, which is not the previously reported benzofuran-2-carbonitrile. The structure of the resulting chromene derivative was confirmed by FT-IR, MS, 1H, 13C NMR and single crystal and powder X-ray diffraction. The reaction pathway under neat conditions (mechanochemical mixing) at ambient temperature was monitored by IR spectral measurements. The versatility of the current green protocol was examined through the reaction of eleven derivatives of o-hydroxybenzaldehyde with malononitrile to obtain 2-amino-3-cyano-4H-chromene derivatives. In addition, malononitrile was further reacted with o-aminobenzaldehydes under neat conditions to yield quinoline derivatives. This journal is © 2012 The Royal Society of Chemistry.

KEYWORDS: Catalyst-free; Catalyst-free synthesis; Chromene derivatives; chromenes; Condensation product; Crystallization process; Malononitriles; Mechanochemicals; Molecular activation; Quinoline derivative; Reaction

pathways; Salicyl aldehyde; Single-crystal and powder; Spectral measurement; Thermal heating, Aldehydes; Mixing; Nuclear magnetic resonance spectroscopy; X ray diffraction, Catalysts

http://pubs.rsc.org/en/content/articlehtml/2012/ra/c2ra21849f

DOI:10.1039/C2RA21849F

147. V. Sinha., J.Williams., J.M.Diesch., F.Drewnick., M.Martinez., H.Harder., E.Regelin, D.Kubistin., H.Bozem., Z.Hosaynali-Beygi., H.Fischer., M.D.Andrés-Hernández., D.Kartal., J.A.Adame., J.Lelieveld (2012) *Constraints on instantaneous ozone production rates and regimes during DOMINO derived using in-situ OH reactivity measurements* .**Atmospheric Chemistry and Physics, 12 (15), pp. 7269-7283.**

ABSTRACT: In this study air masses are characterized in terms of their total OH reactivity which is a robust measure of the "reactive air pollutant loading". The measurements were performed during the DOMINO campaign (Diel Oxidant Mechanisms In relation to Nitrogen Oxides) held from 21/11/2008 to 08/12/2008 at the Atmospheric Sounding Station-El Arenosillo (37.1° N-6.7° W, 40 m a.s.l.). The site was frequently impacted by marine air masses (arriving at the site from the southerly sector) and air masses from the cities of Huelva (located NW of the site), Seville and Madrid (located NNE of the site). OH reactivity values showed strong wind sector dependence. North eastern "continental" air masses were characterized by the highest OH reactivities (average: 31.4 ± 4.5 s -1 range of average diel values: 21.3-40.5 s -1), followed by north western "industrial" air masses (average: 13.8 ± 4.4 s -1; range of average diel values: 7-23.4 s -1) and marine air masses (average: 6.3 ± 6.6 s -1; range of average diel values: below detection limit g-21.7 s -1), respectively. The average OH reactivity for the entire campaign period was ~18 s -1 and no pronounced variation was discernible in the diel profiles with the exception of relatively high values from 09:00 to 11:00 UTC on occasions when air masses arrived from the north western and southern wind sectors. The measured OH reactivity was used to constrain both diel instantaneous ozone production potential rates and regimes. Gross ozone production rates at the site were generally limited by the availability of NOx with peak values of around 20 ppbV O3 h -1. Using the OH reactivity based approach, derived ozone production rates indicate that if NO x would no longer be the limiting factor in air masses arriving from the continental north eastern sector, peak ozone production rates could double. We suggest that the new combined approach of in-situ fast measurements of OH reactivity, nitrogen oxides and peroxy radicals for constraining instantaneous ozone production rates, could significantly improve analyses of upwind point sources and their impact on regional ozone levels. © 2012 Author(s).

KEYWORDS: air mass; atmospheric pollution; diel variation; nitrogen oxides; ozone, Andalucia; Huelva [Andalucia]; Huelva [Huelva (PRV)]; Madrid [Madrid (ADS/PRV)]; Madrid [Spain]; Sevilla; Seville; Spain

http://www.atmos-chem-phys.net/12/7269/2012/acp-12-7269-2012.html

doi:10.5194/acp-12-7269-2012

148. Rishi Raj Trivedi., Samarjit Bhattacharyya (2012) *Constitutive internalization and recycling of metabotropic glutamate receptor 5 (mGluR5)*. **Biochem Biophys Res Commun. 427 (1); page: 185-190.**

ABSTRACT : Ligand-dependent and ligand-independent endocytic trafficking of G-protein coupled receptors (GPCRs) is critical for accurate receptor-mediated signaling and its regulation. Metabotropic glutamate receptor 5 (mGluR5) is a GPCR that plays a crucial role in circuit formation in the brain and also in various forms of synaptic plasticity including learning and memory. Outside the central nervous system this receptor also plays very important role in various other non-neuronal cells like heart cells, skin cells, hepatocytes, etc. Although the ligand-mediated endocytosis of mGluR5 has been studied in some detail, ligand-independent/constitutive endocytosis of the receptor has not been properly studied. Here, we have investigated the constitutive endocytosis of mGluR5 and also the sub-cellular fate of the receptor subsequent to internalization. We show here that mGluR5 undergoes constitutive internalization in HEK293 cells. Following endocytosis, the receptor enters the recycling compartment and no localization of the receptor was observed in the lysosome. In addition, we also report here that most of the receptors recycle to the cell surface subsequent to constitutive internalization. Thus, our data demonstrate that mGluR5 receptors internalize without the application of ligand and the internalized receptors recycle back to the cell surface following constitutive endocytosis.

KEYWORDS: Endocytic trafficking; Recycling; GPCR; Metabotropic glutamate receptor; Glutamate; Neurotransmitter receptor

http://www.sciencedirect.com/science/article/pii/S0006291X12017809

http://dx.doi.org/10.1016/j.bbrc.2012.09.040,

149. Bodhisatta Nandy., Abhilasha Joshi., Zeeshan Syed Ali.**, Sharmi Sen., Nagraj Guru Prasad (2012)** *Degree of adaptive male mate choice is positively correlated with female quality variance .* S**cientific Reports, 2, art. no. 447,**

ABSTRACT: When the cost of reproduction for males and variance in female quality are high, males are predicted to show adaptive mate choice. Using Drosophila melanogaster, we test this prediction and show that sperm limited males preferentially mated with young and/or well fed females. The preferred females had higher reproductive output direct evidence of adaptive precopulatory male mate choice. Our most striking finding is the strong positive correlation between the degree of mating bias showed by the males and the variance in the fitness of the females. We discuss the possible mechanism for such adaptive male mate choice and propose that such choice has important consequences with respect to the existing understanding of the mating system and the evolution of aging.

http://www.nature.com/srep/2012/120608/srep00447/full/srep00447.html?WT.ec_id=SREP-20120612

doi:10.1038/srep00447

150. M.D.Andrés-Hernández., D.Kartal., J.N.Growley., V.**Sinha.**, E.Regelin., M.Martínez-Harder., V.Nenakhov., J.Williams., H.Harder., H.Bozem., W.Song., J.Thieser., M.-J.Tang., Z.Hosaynali Beygi., J.P.Burrows **(2012)** *Diel peroxy radicals in a semi industrial coastal area: nighttime formation of free radicals,* **Atmos. Chem. Phys. Discuss., 12, 19529-19570**

ABSTRACT: : Peroxy radicals were measured by a PeRCA (Peroxy Radical Chemical Amplifier) instrument in the boundary layer during the DOMINO (Diel Oxidant Mechanisms In relation to Nitrogen Oxides) campaign at a coastal, forested site influenced by urban-industrial emissions in Southern Spain in late autumn. Total peroxy radicals ($RO_2^* = HO_2 + \Sigma RO_2$) generally showed a daylight maximum between 10 and 50 pptv at 13:00UTC, with an average of 18 pptv over the 15 days of measurements. Emissions from the industrial area of Huelva often impacted the measurement site at night during the campaign. The processing of significant levels of anthropogenic organics leads to an intense nocturnal radical chemistry accompanied by formation of organic peroxy radicals at comparable levels to those of summer photochemical conditions with peak events up to 60–80 pptv. The RO_2 production initiated by reactions of NO_3 with organic trace gases was estimated to be significant but not sufficient to account for the concentrations of RO_2^* observed in air masses carrying 15 high pollutant loading. The nocturnal production of peroxy radicals seems therefore to be dominated by ozonolysis of volatile organic compounds. RO_2^* diurnal variations were consistent with other HO_2 measurements available at the site. HO_2/RO_2^* ratios generally varied between 0.3 and 0.4 in all wind directions. Occasional $HO_2/RO_2^* \geq 1$ seemed to be associated with periods of high RO_2^* variability and with RO_2 interferences in the HO_2 measurement in air masses with high RO_2 load.
http://www.atmos-chem-phys-discuss.net/12/19529/2012/acpd-12-19529-2012.html
doi:10.5194/acpd-12-19529-2012

151. Matsyendranath Shukla., Kavita Dorai (2012) *Disentangling diffusion information of individual components in a mixture with a 3D COMPACT-IDOSY NMR experiment.* **Magnetic Resonance in Chemistry 50 (5) , pp. 341-346**

ABSTRACT: A new 3D diffusion-ordered heteronuclear NMR experiment COMPACT-IDOSY (cross-polarization optimized multisite polarized accelerated time internally encoded diffusion ordered spectroscopy) has been designed and experimentally implemented on a mixture of flavonoids rutin and quercetin. The pulse sequence uses a cross-polarization mixing period and diffusion encoding gradients internally incorporated into the coherence transfer interval of a long-range heteronuclear correlation experiment. Substantial reduction in experimental time, good sensitivity and excellent resolution of signal overlap lead to the accurate determination of translational diffusion coefficients of individual components in the mixture.

KEYWORDS: DOSY;3D heteronuclear pulse sequence;HMBC;Diffusion *coefficients.*

http://onlinelibrary.wiley.com/doi/10.1002/mrc.2877/full

DOI: 10.1002/mrc.2877

152. Kushal Kr. Banerjee., Champakali Ayyub., **Syed Zeeshan Ali.**, Vinesh Mandot., **Nagaraj G. Prasad.,** Ullas Kolthur-Seetharam (**2012**) *DSir2 in the Adult Fat Body, but Not in Muscles, Regulates Life Span in a Diet-Dependent Manner*.Cell Reports, 2 (6), pp. 1485-1491.

ABSTRACT: Sir2, an evolutionarily conserved NAD+-dependent deacetylase, has been implicated as a key factor in mediating organismal life span. However, recent contradictory findings have brought into question the role of Sir2 and its orthologs in regulating organismal longevity. In this study, we report that Drosophila Sir2 (dSir2) in the adult fat body regulates longevity in a diet-dependent manner. We used inducible Gal4 drivers to knock down and overexpress dSir2 in a tissue-specific manner. A diet-dependent life span phenotype of dSir2 perturbations (both knockdown and overexpression) in the fat body, but not muscles, negates the effects of background genetic mutations. In addition to providing clarity to the field, our study contrasts the ability of dSir2 in two metabolic tissues to affect longevity. We also show that dSir2 knockdown abrogates fat-body dFOXO-dependent life span extension. This report highlights the importance of the interplay between genetic factors and dietary inputs in determining organismal life spans. Using Drosophila, Kolthur-Seetharam and colleagues show that dSir2 in the metabolically relevant tissue of the adult fat body affects organismal life span in a diet-dependent manner. Although fat-body-specific dSir2 knockdown abolishes dietary restriction (DR)-mediated life-

span extension, its overexpression mimics the effect of DR on longevity. The dSir2-dependent longevity phenotype is limited to conditions that lead to an increase in both its own expression and NAD+ levels. The data also indicate that fat-body dSir2 is indispensable for dFOXO-dependent life-span extension.© 2012 The Authors.

KEYWORDS: silent information regulator protein 2; transcription factor FOXO; transcription factor GAL4, adipose tissue; animal experiment; animal tissue; article; controlled study; diet; Drosophila; female; gene mutation; gene overexpression; gene silencing; heredity; imago; lifespan; longevity; muscle tissue; nonhuman; orthology; phenotype; priority journal; tissue specificity

http://www.sciencedirect.com/science/article/pii/S2211124712003944

http://dx.doi.org/10.1016/j.celrep.2012.11.013

153. Rajesh Kochhar (2012) *Early modern natural history: Contributions from the Americas and India*. **Journal of Biosciences, 37 (1) pp. 937-947**. © 2012 Indian Academy of Sciences.

KEYWORDS: India; medical botany; natural history; scientific botany; the Americas

http://link.springer.com/article/10.1007%2Fs12038-012-9272-9

DOI 10.1007/s12038-012-9272-9

154. George Thomas., Ramandeep S. Johal (2012) *Expected behavior of quantum thermodynamic machines with prior information*.**Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 85 (4), art. no. 041146, .**

ABSTRACT: We estimate the expected behavior of the quantum model of a heat engine when we have incomplete information about external macroscopic parameters such as the magnetic field controlling the intrinsic energy scales of the working medium. We explicitly derive the prior probability distribution for these unknown parameters a i(i=1,2). Based on a few simple assumptions, the prior probability distribution is found to be of the form Π(a i) 1/a i. By calculating the expected values of various physical quantities related to this engine, we find that the expected behavior of the quantum model exhibits thermodynamiclike features. This leads us to a surprising proposal that incomplete information quantified as an appropriate prior distribution can lead us to expect classical thermodynamic behavior in quantum models. © 2012 American Physical Society.

KEYWORDS: Classical thermodynamics; Expected values; Incomplete information; Intrinsic energy; Macroscopic parameters; Physical quantities; Prior distribution; Prior information; Quantum models; Quantum thermodynamics; Unknown parameters; Working medium, Heat engines; Magnetic fields, Probability distributions

http://pre.aps.org/abstract/PRE/v85/i4/e041146

DOI:10.1103/PhysRevE.85.041146

155. Pushpender Kumar Sharma., Rajender Kumar., Rakesh Kumar., Owais Mohammad., Ranvir Singh, Jagdeep Kaur **(2012)** *Engineering of a metagenome derived lipase toward thermal tolerance: Effect of asparagine to lysine mutation on the protein surface* . **Gene, 491 (2), pp. 264-271.**

ABSTRACT: A highly thermostable mutant lipase was generated and characterized. Mutant enzyme demonstrated 144 fold enhanced thermostability over the wild type enzyme at 60°C. Interestingly, the overall catalytic efficiency (k cat/K m) of mutant was also enhanced (~20 folds). Circular dichroism spectroscopy, studied as function of temperature, demonstrated that the mutant lipase retained its secondary structure up to 70-80°C, whereas wild type protein structure was completely distorted above 35°C. Additionally, the intrinsic tryptophan fluorescence (a probe for the tertiary structure) also displayed difference in the conformation of two enzymes during temperature dependent unfolding. Furthermore, mutation N355K resulted in extensive H-bonding (Lys355 HZ1OE2 Glu284) with a distance 2.44Å. In contrast to this, Wt enzyme has not shown such H-bonding interaction. © 2011 Elsevier B.V.

KEYWORDS: asparagine; DNA; hydrogen; lysine; triacylglycerol lipase; tryptophan, article; biochemistry; catalysis; circular dichroism; controlled study; enzyme activity; enzyme conformation; enzyme stability; fluorescence spectroscopy; gene mutation; genetic engineering; heat tolerance; hydrogen bond; metagenome; metagenomics; molecular interaction; molecular model; polymerase chain reaction; priority journal; protein expression; protein purification; protein secondary structure; protein tertiary structure; surface property; temperature dependence; thermostability, Amino Acid Substitution; Animals; Asparagine; Circular Dichroism; Enzyme Stability; Lipase; Lysine; Metagenome; Protein Conformation; Protein Folding; Temperature

http://www.sciencedirect.com/science/article/pii/S0378111911005518

http://dx.doi.org/10.1016/j.gene.2011.09.028

156. **Rajesh Kochhar (2012)**. *Fellow of the Royal Astronomical Society.* **Current Science, 102 (7), p. 956. (CORRESPONDENCE)**

Rao et al.1 mention that A. V. Nursing Row was elected a Fellow of the Royal Astronomical Society in 1870. They go on to claim that 'he was the first Indian to be elected Fellow and not Ragoonatha Chary as earlier mentioned by Rao et al.2'. This is some improvement, but not enough. It is a matter of public record that the first Indian to be elected Fellow of the Royal 956 Astronomical Society was Radhanath Sickdhar (his spellings), in 1853.

http://www.currentscience.ac.in/php/toc.php?vol=102&issue=07

157. Visakhi . P (2012) Federated Search Engine : tool for Web Scale e-resource Management in libraries .***In*** : **Next Generation Librarianship: Strategies for change management,** (Ed.) L.S Ramaiah, K.Veeranjaneyulu and G. Sujatha.B.S.Publications, 184-196pp.,

ABSTRACT: The libraries are blessed with latest technology and information boom. Due to this advancements, the libraries have become more vulnerable to the users with challenges of effective single dynamic search interface for

providing effective , up-to-date , accurate , relevant and instant infiormation to its patron from multiple databases of library subscribed / Open access sources. The concept of “ federated search engine and its historical developments , its functiong mechanism was discussed. Its features, merits and flaws over “ Web search ebgines” were also part of the discussion.The merits and flaws of some of free and commecrcial federated search engines over the other were also highlighted.

*http://www.bookadda.com/books/next-generation-librarianship-strategies-*change-8178002655-9788178002651

ISBN: 9788178002651

158. E.Harris., **B.Sinha.,** P.Hoppe., S.Foley., S.Borrmann (**2012**).: *Fractionation of sulfur isotopes during heterogeneous oxidation of SO2 on sea salt aerosol: A new tool to investigate non-sea salt sulfate production in the marine boundary layer*. **Atmospheric Chemistry and Physics, 12, PP. 2707- 2742**

ABSTRACT: The oxidation of SO_2 to sulfate on sea salt aerosols in the marine environment is highly important because of its effect on the size distribution of sulfate and the potential for new particle nucleation from H_2SO_4 (g). However, models of the sulfur cycle are not currently able to account for the complex relationship between particle size, alkalinity, oxidation pathway and rate – which is critical as SO_2 oxidation by O_3 and Cl catalysis are limited by aerosol alkalinity, whereas oxidation by hypohalous acids and transition metal ions can continue at low pH once alkalinity is titrated. We have measured $^{34}S/^{32}S$ fractionation factors for SO_2 oxidation in sea salt, pure water and NaOCl aerosol, as well as the pH dependency of fractionation. Oxidation of SO_2 by NaOCl aerosol was extremely efficient, with a reactive uptake coefficient of ~0.5, and produced sulfate that was enriched in ^{32}S with $\alpha_{OCl} = 0.9882 \pm 0.0036$ at 19 °C. Oxidation on sea salt aerosol was much less efficient than on NaOCl aerosol, suggesting alkalinity was already exhausted on the short timescale of the experiments. Measurements at pH = 2.1 and 7.2 were used to calculate fractionation factors for each step from $SO_2(g) \rightarrow$ multiple steps $\rightarrow SO_2^{-3}$. Oxidation on sea salt aerosol resulted in a lower fractionation factor than expected for oxidation of SO_2^{-3} by O_3 ($\alpha_{seasalt} = 1.0124 \pm 0.0017$ at 19 °C).

Comparison of the lower fractionation during oxidation on sea salt aerosol to the fractionation factor for high pH oxidation shows HOCl contributed 29% of S(IV) oxidation on sea salt in the short experimental timescale, highlighting the potential importance of hypohalous acids in the marine environment. The sulfur isotope fractionation factors measured in this study allow differentiation between the alkalinity-limited pathways – oxidation by O3 and by Cl catalysis (α_{34} =1.0163±0.0018 at 19 °C in pure water or 1.0199±0.0024 at pH = 7.2) – which favour the heavy isotope, and the alkalinity non-limited pathways – oxidation by transition metal catalysis (α_{34} = 0.9905±0.0031 at 19 °C, Harris et al., 2012a) and by hypohalites (α_{34} = 0.9882±0.0036 at 19 °C) – which favour the light isotope. In combination with field measurements of the oxygen and sulfur isotopic composition of SO_2 and sulfate, the fractionation factors presented in this paper may be capable of constraining the relative importance of different oxidation pathways in the marine boundary layer.

KEYWORDSs: nonmetal redox kinetics; size distribution; atlantic-ocean; acid reactions; particles; chemistry; ozone; model; nanosims; seawater

http://www.atmos-chem-phys-discuss.net/12/2707/2012/acpd-12-2707-2012.html

doi:10.5194/acpd-12-2707-2012

159. Inder Bir S. Passi (2012) *Group algebras .* **Indian Journal of Pure and Applied Mathematics, 43 (2), pp. 89-106.**

ABSTRACT: Given a group G and a commutative ring k with identity, one can define an k-algebra k[G] called the group algebra of G over k. An element α k[G] is said to be algebraic if f(α) = 0 for some non-zero polynomial f(X) k[X]. We will discuss some of the developments in the study of algebraic elements in group algebras. © 2012 The Indian National Science Academy.

KEYWORDS: algebraic elements; augmentation ideal; Bass conjecture; dimension sub-groups; Group algebras; idempotents; Jordan decomposition; partial augmentation

http://link.springer.com/article/10.1007%2Fs13226-012-0006-3

160. Hardeep Kaur., Dwaipayan Ganguli., **Anand K. Bachhawat (2012)** *Glutathione degradation by the alternative pathway (DUG pathway) in Saccharomyces cerevisiae is initiated by (Dug2p-Dug3p)2 complex, a novel glutamine amidotransferase (GATase) enzyme acting on glutathione*.**Journal of Biological Chemistry, 287 (12), pp. 8920-8931.**

ABSTRACT: The recently identified, fungi-specific alternative pathway of glutathione degradation requires the participation of three genes, DUG1, DUG2, and DUG3. Dug1p has earlier been shown to function as a Cys-Gly-specific dipeptidase. In the present study, we describe the characterization of Dug2p and Dug3p. Dug3p has a functional glutamine amidotransferase (GATase) II domain that is catalytically important for glutathione degradation as demonstrated through mutational analysis.Dug2p,whichhasan N-terminal WD40 and a C-terminal M20A peptidase domain, has no peptidase activity. The previously demonstrated Dug2p-Dug3p interaction was found to be mediated through the WD40 domain of Dug2p. Dug2p was also shown to be able to homodimerize, and this was mediated by itsM20Apeptidase domain. In vitro reconstitution assays revealed that Dug2p and Dug3p were required together for the cleavage of glutathione into glutamate and Cys-Gly. Purification through gel filtration chromatography confirmed the formation of aDug2p-Dug3pcomplex.Thefunctionalcomplex had a molecular weight that corresponded to (Dug2p-Dug3p) 2 in addition to higher molecular weight oligomers and displayed Michaelis-Menten kinetics.(Dug2p-Dug3p) 2hadaK mfor glutathione of 1.2 mM, suggesting a novel GATase enzyme that acted on glutathione. Dug1p activity in glutathione degradation was found to be restricted to its Cys-Gly peptidase activity, which functioned downstream of the (Dug2p-Dug3p) 2 GATase. The DUG2 and DUG3genes, but notDUG1, were derepressed by sulfur limitation. Based on these studies and the functioning of GATases, a mechanism is proposed for the functioning of the Dug proteins in the degradation of glutathione. © 2012 by The American Society for Biochemistry and Molecular Biology, Inc.

KEYWORDS: Gel-filtration chromatography; Glutathiones; Homodimerize; In-vitro; Michaelis-Menten kinetic; N-terminals; Peptidase activity; Reconstitution assay; Sulfur limitation, Amino acids; Degradation; Enzymes; Gel permeation chromatography; Genes; Molecular weight; Oligomers; Yeast, Peptides, cysteinylglycine; fungal protein; glutamic acid; glutamine amidotransferase;

glutathione; protein Dug1; protein Dug2; protein Dug2p; protein Dug3; protein Dug3p; sulfur; transferase; unclassified drug, article; catalysis; complex formation; controlled study; dimerization; DUG1 gene; DUG2 gene; DUG3 gene; enzyme activity; enzyme assay; enzyme purification; Escherichia coli; fungal gene; fungal metabolism; gel filtration chromatography; in vitro study; Michaelis Menten kinetics; molecular weight; mutational analysis; nonhuman; nutrient limitation; priority journal; protein degradation; protein domain; protein function; protein protein interaction; Saccharomyces cerevisiae; signal transduction, Amino Acid Sequence; Carbon-Nitrogen Ligases; Dipeptidases; Glutamic Acid; Glutathione; Kinetics; Molecular Sequence Data; Peptide Hydrolases; Protein Structure, Tertiary; Saccharomyces cerevisiae; Saccharomyces cerevisiae Proteins; Sequence Homology, Amino Acid; Substrate Specificity; Sulfur; Transaminases, Fungi; Saccharomyces cerevisiae

http://www.jbc.org/content/287/12/8920.short

161. Rajeev Kapri (2012) *Hysteresis and nonequilibrium work theorem for DNA unzipping* Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, 86 (4), art. no. 041906, .

ABSTRACT: We study by using Monte Carlo simulations the hysteresis in unzipping and rezipping of a double stranded DNA (dsDNA) by pulling its strands in opposite directions in the fixed force ensemble. The force is increased at a constant rate from an initial value g 0 to some maximum value g m that lies above the phase boundary and then decreased back again to g 0. We observed hysteresis during a complete cycle of unzipping and rezipping. We obtained probability distributions of work performed over a cycle of unzipping and rezipping for various pulling rates. The mean of the distribution is found to be close (the difference being within 10%, except for very fast pulling) to the area of the hysteresis loop. We extract the equilibrium force versus separation isotherm by using the work theorem on repeated nonequilibrium force measurements. Our method is capable of reproducing the equilibrium and the nonequilibrium force-separation isotherms for the spontaneous rezipping of dsDNA. © 2012 American Physical Society.

KEYWORDS: Constant rate; DNA unzipping; Double-stranded DNA (ds-DNA); Equilibrium forces; Initial values; Maximum values; Monte Carlo Simulation; Non equilibrium; Nonequilibrium work; Pulling rates, Isotherms; Monte Carlo methods; Probability distributions; Separation, Hysteresis

http://link.aps.org/doi/10.1103/PhysRevE.86.041906
DOI: 10.1103/PhysRevE.86.041906

162. Nayyar Ahmad Aslam., Vadla Rajkumar., Chennakesava Reddy., Makoto Yasuda, Akio Baba.**, Srinivasarao Arulananda Babu (2012)** *Indium-mediated addition of γ-substituted allylic halides to N-aryl α-imino esters: Diastereoselective production of β,β′- disubstituted α-amino acid derivatives with two contiguous stereocenters* . **European Journal of Organic Chemistry, (23), pp. 4395-4411.**

ABSTRACT: Chelation-controlled Barbier-type indium-mediated addition of γ-substituted allylic halides to N-aryl (including N-PMP) α-imino- and N-acylhydrazono esters and highly diastereoselective tailoring of functionalized γ,δ-unsaturated β,β'-disubstituted N-aryl α-amino acid derivatives, bearing two contiguous stereocenters is reported. Further N-allylation of the resulting γ,δ-unsaturated β,β'-disubstituted N-aryl amino acid derivatives followed by ring closing metathesis (RCM) led to the synthesis of 2,3-disubstituted N-aryltetrahydropyridine derivatives bearing two contiguous stereocenters. The stereochemistry of the key products was unequivocally established from X-ray structure analyses. Highly diastereoselective C-C bond formation through Barbier-type indium-mediated addition of γ-substituted allylic halides to N-aryl α-imino and α-hydrazono esters was established. Diastereoselective production of γ,δ-unsaturated β,β'-disubstituted N-aryl (including N-PMP) α-amino acid- and 2,3-disubstituted N-aryltetrahydropyridine derivatives bearing two contiguous stereocenters was accomplished. Copyright © 2012 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

KEYWORDS: Allylation; Amino acids; Diastereoselectivity; Indium; Synthetic methods

http://onlinelibrary.wiley.com/doi/10.1002/ejoc.201200254/full

DOI: 10.1002/ejoc.201200254

163. George Thomas., Preety Aneja., Ramandeep S Johal(2012) *Informative priors and the analogy between quantum and classical heat engines* . **Physica Scripta, (T151), art. no. 014031**, .

ABSTRACT: When incomplete information about the control parameters is quantified as a prior distribution, a subtle connection emerges between quantum heat engines and their classical analogues. We study the quantum model where the uncertain parameters are the intrinsic energy scales and compare it with the classical models where the intermediate temperature is the uncertain parameter. The prior distribution quantifying the incomplete information has the form $\pi(x)\propto 1/x$ in both the quantum and the classical models. The expected efficiency calculated in the near-equilibrium limit approaches the value of one third of Carnot efficiency. © 2012 The Royal Swedish Academy of Sciences.

KEYWORDS: Carnot efficiency; Classical model; Control parameters; Incomplete information; Informative Priors; Intermediate temperatures; Intrinsic energy; Limit approach; Prior distribution; Quantum heat engines; Quantum models; Uncertain parameters, Molecular physics; Physics, Chaotic systems

http://arxiv.org/abs/1205.0667

http://iopscience.iop.org/1402-4896/2012/T151/014031

doi:10.1088/0031-8949/2012/T151/014031

164. Uzma Fatima., Balvinder Singh., Karthikeyan Subramanian., **Purnananda Guptasarma (2012)** *Insufficient (sub-native) helix content in soluble/solid aggregates of recombinant and engineered forms of IL-2 throws light on how aggregated IL-2 is biologically active* .**Protein Journal, 31 (7), pp. 529-543.**

ABSTRACT: Interleukin 2 (IL-2) is an extremely aggregation-prone, all-alpha helical cytokine. In its receptor-bound state, ~72 % of the polypeptide chain adopts helical structure and there is no beta sheet content whatsoever. In the past, recombinant IL-2 has been formulated and used therapeutically in humans, following production in E. coli. Therapeutic IL-2 consists entirely of functionally-active soluble aggregates with ~30 subunits per aggregate particle. Side-effects attributed to aggregation resulted in discontinuation of usage over a decade ago. Structurally, and biochemically, activity in IL-2 aggregates can potentially be explained in one of two ways: (a) individual IL-2 chains exist in sterically-accessible, receptor binding-competent (native) structures, allowing aggregates to bind directly to IL-2 receptors (IL-2R); alternatively, (b) IL-2 chains dissociate from aggregates, become free to adopt native structure, and then bind to IL-2R. We produced native IL-2 and numerous engineered forms in E. coli with the objective of obtaining insights into these possibilities. Each IL-2 variant was subjected to size exclusion chromatography, circular dichroism (CD) and Fourier transform infrared spectroscopy (FTIR). All forms produced and studied (including those with native IL-2 sequences) turned out to aggregate and also display less than ~50 % helix content as well as significant beta sheet content. No conditions were found that obviate aggregation. Aggregated IL-2 is thus insufficiently native-like to bind to IL-2R. Activity in aggregates thus probably owes to adoption of receptor binding-competent structures by chains that have already dissociated from aggregates. © 2012 Springer Science+Business Media, LLC.

KEYWORDS: interleukin 2; interleukin 2 receptor; recombinant interleukin 2, article; circular dichroism; glycosylation; infrared spectroscopy; protein binding; protein folding; protein structure

http://link.springer.com/article/10.1007/s10930-012-9429-2/fulltext.html

DOI: 10.1007/s10930-012-9429-2

165. Kuljeet Singh Sandhu., Guoliang Li, Huay Mei Poh., Yu Ling Kelly Quek., Yee Yen Sia., Su Qin Peh., Fabianus Hendriyan Mulawadi., Joanne Lim., Mile Sikic, Francesca Menghi., Anbupalam Thalamuthu., Wing Kin Sung., Xiaoan Ruan., Melissa Jane Fullwood., Edison Liu., Peter Csermely., Yijun Ruan.**(2012)** *Large-Scale Functional Organization of Long-Range Chromatin Interaction Networks*. **Cell Reports, 2 (5), pp. 1207-1219.**

ABSTRACT: Chromatin interactions play important roles in transcription regulation. To better understand the underlying evolutionary and functional constraints of these interactions, we implemented a systems approach to examine RNA polymerase-II-associated chromatin interactions in human cells. We found that 40% of the total genomic elements involved in chromatin interactions converged to a giant, scale-free-like, hierarchical network organized into chromatin communities. The communities were enriched in specific functions and were syntenic through evolution. Disease-associated SNPs from genome-wide association studies were enriched among the nodes with fewer interactions, implying their selection against deleterious interactions by limiting the total number of interactions, a model that we further reconciled using somatic and germline cancer mutation data. The hubs lacked disease-associated SNPs, constituted a nonrandomly interconnected core of key cellular functions, and exhibited lethality in mouse mutants, supporting an evolutionary selection that favored the nonrandom spatial clustering of the least-evolving key genomic domains against random genetic or transcriptional errors in the genome. Altogether, our analyses reveal a systems-level evolutionary framework that shapes functionally compartmentalized and error-tolerant transcriptional regulation of human genome in three dimensions. It is becoming increasingly clear that genes are not autonomous transcriptional units; instead, they physically interact with one another to coordinate transcriptional regulation. Using a network approach, Ruan and colleagues unravel an evolutionarily constrained systems organization of transcription-associated chromatin in the human genome. Their observations provide a possible chromatin-level explanation for how disease-associated mutations evolve and how key cellular genes escape genetic and transcriptional errors. © 2012 The Authors.

KEYWORDS: RNA polymerase II, article; chromatin assembly and disassembly; evolution; gene mutation; human; human cell; human genome; priority journal; single nucleotide polymorphism; somatic mutation; synteny; transcription regulation, Margarodidae

http://www.sciencedirect.com/science/article/pii/S2211124712003269

http://dx.doi.org/10.1016/j.celrep.2012.09.022

166. Ramarao Parella., Naveen., Srinivasarao Arulananda Babu (2012) *Magnetic nano Fe_3O_4 and $CuFe_2O_4$ as heterogeneous catalysts: A green method for the stereo- and regioselective reactions of epoxides with indoles/pyrroles*. Catalysis Communications, 29, pp. 118-121.

ABSTRACT: In this paper, we report a new solvent-free catalytic method using the magnetic nano Fe_3O_4 and $CuFe_2O_4$ as competent heterogeneous catalysts for the stereo- and regioselective reactions of epoxides with indoles/pyrroles, which gave the C-alkylated indoles/pyrroles. Chiral epoxides gave the alkylated indoles with a complete inversion of stereochemistry. © 2012 Elsevier B.V.

KEYWORDS: C-C bond formation; Chiral epoxides; Epoxides; Green method; Heterocycles; Heterogeneous catalyst; Nano-Fe; Regioselective reactions; Solvent free, Nanoparticles; Stereochemistry, Regioselectivity

http://www.sciencedirect.com/science/article/pii/S156673671200369X

http://dx.doi.org/10.1016/j.catcom.2012.09.030,

167. Remo Storni., Hiroyasu Ando, Kazuyuki Aihara., K. Murali., **Sudeshna Sinha (2012)** *Manipulating potential wells in Logical Stochastic Resonance to obtain XOR logic.* **Physics Letters, Section A: General, Atomic and Solid State Physics, 376 (8-9), pp. 930-937.**

ABSTRACT: Logical Stochastic Resonance (LSR) is the application of Stochastic Resonance to logic computation, namely the phenomenon where a nonlinear system driven by weak signals representing logic inputs, under optimal noise, can yield logic outputs. We extend the existing results, obtained in the context of bistable systems, to multi-stable dynamical systems, allowing us to obtain XOR logic, in addition to the AND (NAND) and OR (NOR) logic observed in earlier studies. This strategy widens the scope of LSR from the application point of view, as XOR forms the basis of ubiquitous bit-by-bit addition, and conceptually, showing the ability to yield non-monotonic input-output logic associations. © 2012 Elsevier B.V. All rights reserved.

KEYWORDS: Alternate computation; Logic gate; Stochastic Resonance

http://www.sciencedirect.com/science/article/pii/S0375960111015027

http://dx.doi.org/10.1016/j.physleta.2011.12.036,

168. Abhishek Khanna., Ramandeep S. Johal (2012) *Maximum power point characteristics of generalized heat engines with finite time and finite heat capacities.* **Journal of Thermodynamics, 1 (1), art. no. 246914, .**

ABSTRACT: We revisit the problem of optimal power extraction in four-step cycles (two adiabatic and two heat-transfer branches) when the finite-rate heat transfer obeys a linear law and the heat reservoirs have finite heat capacities. The heat-transfer branch follows a polytropic process in which the heat capacity of the working fluid stays constant. For the case of ideal gas as working fluid and a given switching time, it is shown that maximum work is obtained at Curzon-Ahlborn efficiency. Our expressions clearly show the dependence on the relative magnitudes of heat capacities of the fluid and the reservoirs. Many previous formulae, including infinite reservoirs, infinite-time cycles, and Carnot-like and non-Carnot-like cycles, are recovered as special cases of our model. © 2012 Abhishek Khanna and Ramandeep S. Johal.

http://www.hindawi.com/journals/jtd/2012/246914
doi:10.1155/2012/246914

169. Gianluca Giovannetti., **Sanjeev Kumar.**, Carmine Ortix., Massimo Capone., Jeroen van den Brink **(2012)** *Microscopic origin of large negative magnetoelectric coupling in Sr1/2Ba1/2MnO$_3$* . **Physical Review Letters, 109 (10), art. no. 107601, ABSTRACT:** With a combined ab initio density functional and model Hamiltonian approach we establish that in the recently discovered multiferroic phase of the manganite Sr 1/2Ba 1/2MnO$_3$ the polar distortion of Mn and O ions is stabilized via enhanced in-plane Mn-O hybridizations. The magnetic superexchange interaction is very sensitive to the polar bond-bending distortion, and we find that this dependence directly causes a strong magnetoelectric coupling. This novel mechanism for multiferroicity is consistent with the experimentally observed reduced ferroelectric polarization upon the onset of magnetic ordering. © 2012 American Physical Society.

KEYWORDS: Ab initio; Density functionals; Ferroelectric polarization; Magnetoelectric couplings; Model Hamiltonians; Multiferroics; Polar distortion; Superexchange interaction, Electromagnetic coupling; Manganese, Manganese oxide

http://prl.aps.org/abstract/PRL/v109/i10/e107601

DOI:10.1103/PhysRevLett.109.107601

170. Pushpender Kumar Sharma., Monika Sharma, Jagdeep Kaur (**2012**) *Metagenomic approach to explore microbial diversity and genetic potential of uncultured microorganisms from different environment niches.* **Research Journal of Pharmaceutical, Biological and Chemical Sciences, 3 (2), pp. 947-956.**

ABSTRACT: The term metagenomics refers to genomic analysis of those microorganisms, which are difficult to cultivate in standard cultivation medium. The 16S rRNA study from various environments has provided a strong evidence for the existence of uncultured microorganism. The novel genes and gene products discovered by metagenomic approach include many hydrolytic enzymes, novel molecules and antimicrobial compounds. Furthermore, metagenomic studies from various extreme environments shed light into genomic diversity and existence of various co-operations among the microorganisms. This review discusses the concepts, basic tools and applications of metagenomic gene cloning in discovering novel molecules and microbial diversities. In addition to this, this review also highlights the impact of uncultured microorganisms on human health and environment.

KEYWORDS: RNA 16S; triacylglycerol lipase, biocatalyst; ecological niche; gene library; genetic variability; genome analysis; metagenomics; microbial activity; microbial community; microbial diversity; microbial genetics; molecular cloning; nonhuman; polymerase chain reaction; review; RNA analysis; RNA sequence; species richness

http://www.rjpbcs.com/pdf/2012_3%282%29/%5B110%5D.pdf

171. Shilpa Setia., Sumyra Sidiq., Santanu Kumar Pal (**2012**) *Microwave-assisted synthesis of novel oligomeric rod-disc hybrids*. **Tetrahedron Letters, 53 (47), pp. 6446-6450.**

ABSTRACT: Microwave-assisted syntheses of five new oligomeric liquid crystals (LC) are reported for the first time consisting of rufigallol-based core attached to which 8-cyanobiphenyl units via flexible alkyl spacers. The synthesis of the target compounds was challenging since classical reactions failed to produce these hybrids. Chemical structures of these hybrids were determined by ^{1}H

NMR, ^{13}C NMR, IR, UV spectroscopy and elemental analysis. The thermotropic liquid crystalline properties of these new compounds were investigated by polarizing optical microscopy (POM), differential scanning calorimetry (DSC) and X-ray diffractometry (XRD). © 2012 Elsevier Ltd. All rights reserved.

KEYWORDS: alkyl group; biphenyl; oligomer, article; carbon nuclear magnetic resonance; chemical reaction; chemical structure; crystal structure; differential scanning calorimetry; infrared spectroscopy; liquid crystal; microscopy; microwave cooking; proton nuclear magnetic resonance; synthesis; ultraviolet spectroscopy; X ray diffraction

http://www.sciencedirect.com/science/article/pii/S0040403912016346

http://dx.doi.org/10.1016/j.tetlet.2012.09.058

172. D.Mogensen., S.Smolander., A.Sogachev., L.Zhou, **V.Sinha.,** A.Guenther,. J.Williams., T.Nieminen., M.K.Kajos., J.Rinne., M.Kulmala, M.Boy **(2012)** *Modelling atmospheric OH-reactivity in a boreal forest ecosystem*. **Atmospheric Chemistry and Physics, 11 (18), pp. 9709-9719.**

ABSTRACT: We have modelled the total atmospheric OH-reactivity in a boreal forest and investigated the individual contributions from gas phase inorganic species, isoprene, monoterpenes, and methane along with other important VOCs. Daily and seasonal variation in OH-reactivity for the year 2008 was examined as well as the vertical OH-reactivity profile. We have used SOSA; a one dimensional vertical chemistry-transport model (Boy et al., 2011a) together with measurements from Hyytiälä, SMEAR II station, Southern Finland, conducted in August 2008. Model simulations only account for ~30-50% of the total measured OH sink, and in our opinion, the reason for missing OH-reactivity is due to unmeasured unknown BVOCs, and limitations in our knowledge of atmospheric chemistry including uncertainties in rate constants. Furthermore, we found that the OH-reactivity correlates with both organic and inorganic compounds and increases during summer. The summertime canopy level OH-reactivity peaks during night and the vertical OH-reactivity decreases with height. © 2011 Author(s) .

KEYWORDS: atmospheric chemistry; atmospheric modeling; boreal forest; canopy; computer simulation; forest ecosystem; volatile organic compound, Finland

http://www.atmos-chem-phys.net/11/9709/2011/acp-11-9709-2011.html

doi:10.5194/acp-11-9709-2011

173. Bindiya Arora., D. K. Nandy ., B. K. Sahoo (**2012**) *Multipolar Black Body Radiation Shifts for the Single Ion BASED Optical frequency standards,Clocks .* **Phys. Rev. A 85, 012506**

ABSTRACT: Appraising the projected `$10^{-18}$` fractional uncertainty in the optical frequency standards using singly ionized ions, we estimate the black-body radiation (BBR) shifts due to the magnetic dipole (M1) and electric quadrupole (E2) multipoles of the magnetic and electric fields, respectively. Mul- tipolar scalar polarizabilities are determined for the singly ionized calcium `(Ca$^+$)` and strontium `(Sr$^+$)` ions using the relativistic coupled-cluster method; though the theory can be exercised for any single ion clock proposal. The expected energy shifts for the respective clock transitions are estimated to be $4.38(3) \times 10^{-4}$ Hz for Ca$^+$ and $9.50(7) \times 10^{-5}$ Hz for Sr$^+$. These shifts are large enough and may be prerequisite for the frequency standards to achieve the foreseen `$10^{-18}$` precision goal.

http://arxiv.org/abs/1108.1639

http://pra.aps.org/abstract/PRA/v85/i1/e012506

174. Manoj Nimbalkar,, Robert Zeier, Jorge L. Neves,, S. Begam Elavarasi,, Haidong Yuan, Navin Khaneja,, **Kavita Dorai,**, Steffen J. Glaser (**2012**) *Multiple-spin coherence transfer in linear Ising spin chains and beyond: numerically-optimized pulses and experiments.* **Physical Review A, 85, 012325**

ABSTRACT : We study multiple-spin coherence transfers in linear Ising spin chains with nearest neighbor couplings. These constitute a model for efficient

information transfers in future quantum computing devices and for many multi-dimensional experiments for the assignment of complex spectra in nuclear magnetic resonance spectroscopy. We complement prior analytic techniques for multiple-spin coherence transfers with a systematic numerical study where we obtain strong evidence that a certain analytically-motivated family of restricted controls is sufficient for time-optimality. In the case of a linear three-spin system, additional evidence suggests that prior analytic pulse sequences using this family of restricted controls are time-optimal even for arbitrary local controls. In addition, we compare the pulse sequences for linear Ising spin chains to pulse sequences for more realistic spin systems with additional long-range couplings between non-adjacent spins. We experimentally implement the derived pulse sequences in three and four spin systems and demonstrate that they are applicable in realistic settings under relaxation and experimental imperfections-in particular-by deriving broadband pulse sequences which are robust with respect to frequency offsets.

http://arxiv.org/abs/1110.5262

http://pra.aps.org/abstract/PRA/v85/i1/e012325

175 . Aridaman Pandit,, Anil Kumar Dasanna,, **Somdatta Sinha (2012)** *Multifractal analysis of HIV-1 genomes* .**Molecular Phylogenetics and Evolution, 62 (2), pp. 756-763.**

ABSTRACT: Pathogens like HIV-1, which evolve into many closely related variants displaying differential infectivity and evolutionary dynamics in a short time scale, require fast and accurate classification. Conventional whole genome sequence alignment-based methods are computationally expensive and involve complex analysis. Alignment-free methodologies are increasingly being used to effectively differentiate genomic variations between viral species. Multifractal analysis, which explores the self-similar nature of genomes, is an alignment-free methodology that has been applied to study such variations. However, whether multifractal analysis can quantify variations between closely related genomes, such as the HIV-1 subtypes, is an open question. Here we address the above by implementing the multifractal analysis on four retroviral genomes (HIV-1, HIV-2, SIVcpz, and HTLV-1), and demonstrate that individual multifractal properties can differentiate between different retrovirus types easily. However, the individual multifractal measures do not resolve within-group variations for different known subtypes of HIV-1 M group. We show here that these known subtypes can instead be classified correctly using a_2 combination of the crucial multifractal measures. This method is simple and computationally fast in comparison to the conventional alignment-based methods for whole genome phylogenetic analysis. © 2011 Elsevier Inc.

KEYWORDS: archaeal genome; archaebacterium; article; classification; genetic variability; genetics; human; Human immunodeficiency virus 1; Human immunodeficiency virus 2; Human T cell leukemia virus 1; multigene family; multivariate analysis; phylogeny; principal component analysis; Simian immunodeficiency virus; species difference; theoretical model; virus genome, Archaea; Genetic Variation; Genome, Archaeal; Genome, Viral; HIV-1; HIV-2; Human T-lymphotropic virus 1; Humans; Models, Theoretical; Multigene Family; Multivariate Analysis; Phylogeny; Principal Component Analysis; Simian immunodeficiency virus; Species Specificity, Human immunodeficiency virus; Human immunodeficiency virus 1; Human immunodeficiency virus 2; Human T-lymphotropic virus

http://www.sciencedirect.com/science/article/pii/S105579031100488X

http://dx.doi.org/10.1016/j.ympev.2011.11.017,

176. R.Comin,, G.Levy,, B.Ludbrook,, Z.-H.Zhu,, C.N.Veenstra,, J.A.Rosen,, **Yogesh Singh,,** P.Gegenwart, D.Stricker,, J.N.Hancock,, D.Van Der Marel,, I.S.Elfimov,, A.Damascelli **(2012)** *Na_2IrO_3 as a novel relativistic mott insulator with a 340-meV gap* . ***Physical Review Letters, 109 (26)*, Art. No. 266406.**

ABSTRACT: We study Na_2IrO_3 by angle-resolved photoemission spectroscopy, optics, and band structure calculations in the local-density approximation (LDA). The weak dispersion of the Ir $5d\text{-}t_{2g}$ manifold highlights the importance of structural distortions and spin-orbit (SO) coupling in driving the system closer to a Mott transition. We detect an insulating gap $\Delta gap \simeq 340$ meV which, at variance with a Slater-type description, is already open at 300 K and does not show significant temperature dependence even across $TN \simeq 15$ K An LDA analysis with

the inclusion of SO and Coulomb repulsion U reveals that, while the prodromes of an underlying insulating state are already found in LDA+SO, the correct gap magnitude can only be reproduced by LDA+SO+U, with U=3 eV. This establishes Na_2IrO_3 as a novel type of Mott-like correlated insulator in which Coulomb and relativistic effects have to be treated on an equal footing. © 2012 American Physical Society.

KEYWORDS: Angle resolved photoemission spectroscopy; Band structure calculation; Coulomb repulsions; Gap magnitude; Insulating gap; Insulating state; Mott insulators; Mott transitions; Relativistic effects; Spin-orbit couplings; Structural distortions; Temperature dependence, Iridium; Photoelectron spectroscopy; Quantum chemistry, Sodium

http://prl.aps.org/abstract/PRL/v109/i26/e266406

DOI: 10.1103/PhysRevLett.109.266406

177. Vijit Dalal,, Mily Bhattacharya,, Dominic Narang,, Pushpender K. Sharma,, Samrat Mukhopadhyay (2012) .*Nanoscale fluorescence imaging of single amyloid fibrils*. **Journal of Physical Chemistry Letters, 3 (13), pp. 1783-1787.**

ABSTRACT: Amyloid formation is implicated in a variety of human diseases. It is important to perform high-resolution optical imaging of individual amyloid fibrils to delineate the structural basis of supramolecular protein assembly. However, amyloid fibrils do not lend themselves to the conventional microscopic resolution, which is hindered by the diffraction limit. Here we show super-resolution fluorescence imaging of fluorescently stained amyloid fibrils derived from disease-associated human β 2-microglobulin using near-field scanning fluorescence microscopy. Using this technique, we were able to resolve the fibrils that were spatially separated by ~75 nm. We have also been able to interrogate individual fibrils in a fibril-by-fibril manner by simultaneously monitoring both nanoscale topography and fluorescence brightness along the length of the fibrils. This method holds promise to detect conformational distributions and heterogeneity that are believed to correlate with the supramolecular packing of misfolded proteins within the fibrils in a diverse conformationally enciphered prion strains and amyloid polymorphs. © 2012 American Chemical Society.

KEYWORDS: Amyloid fibril; Amyloid formation; Conformational distribution; Diffraction limits; Fluorescence imaging; High resolution; Human disease; Microscopic resolution; Misfolded proteins; Nano scale; Nanoscale topography; Near-field scanning; Optical imaging; Protein assembly; Structural basis; Super resolution; Supramolecular packing, Diffraction; Fluorescence; Fluorescence microscopy; Glycoproteins; Nanotechnology; Optical resolving power; Supramolecular chemistry, Proteins

http://pubs.acs.org/doi/abs/10.1021/jz300687f

DOI: 10.1021/jz300687f

178. Maheswararao Karanam., Sagarika Dev., Angshuman Roy Choudhury (2012) *New Polymorphs of Fluconazole: Results from Cocrystallization Experiments.* **Crystal Growth & Design, 12(1), 240-252 .**

ABSTRACT: Fluconazole is known as an antifungal drug since 1983. Its propensity for the formation of new polymorphs and salts has been reported in the literature, mostly by powder X-ray diffraction and solid state Raman spectroscopy. In the present study, we are elucidating the structures of four polymorphs of fluconazole using single crystal X-ray diffraction. Raman spectra of the single crystals of these polymorphs also support our study. These polymorphs were grown in the presence of the cocrystal formers. This indicates that fluconazole interacts with the cocrystal former in the solution, and possibly these interactions result into the generation of new polymorphs of it. These polymorphs of fluconazole exhibit the conformational flexibility of the molecule, and hence we observed seven different conformers of the molecule in the reported polymorphs. Although these forms have strong O–H···N hydrogen bonds, the nature of the packing of the molecules is a cumulative effect of a number of weaker intermolecular forces such as C–H···O, C–H···N, and C–H···F and the strong hydrogen bond.

http://pubs.acs.org/doi/full/10.1021/cg201005y

DOI: 10.1021/cg201005

179. Panjab Arde., B. T. Ramanjaneyulu., Virsinha Reddy., Apurv Saxena., R. Vijaya Anand (**2012**) *N-Heterocyclic Carbene Catalysed Aerobic Oxidation of Aromatic Aldehydes to Aryl Esters using Boronic Acid*s, **Org. Biomol. Chem. 10, 848** -851

ABSTRACT: The organocatalytic behavior of N-heterocyclic carbenes in the aerobic oxidation of aromatic aldehydes to esters with boronic acids has been explored. This transition metal-free protocol allows access to a wide variety of aromatic esters in good to excellent yields under mild *reaction conditions.*

http://pubs.rsc.org/en/content/articlehtml/2012/ob/c1ob06566a

DOI:10.1039/C1OB06566A

180. Vivek Kohar., Sudeshna Sinha (2012) *Noise-assisted morphing of memory and logic function* **Physics Letters, Section A: General, Atomic and Solid State Physics, 376 (8-9), pp. 957-962**.

ABSTRACT: We demonstrate how noise allows a bistable system to behave as a memory device, as well as a logic gate. Namely, in some optimal range of noise, the system can operate flexibly, both as a NAND/AND gate and a Set-Reset latch, by varying an asymmetrizing bias. Thus we show how this system implements memory, even for sub-threshold input signals, using noise constructively to store information. This can lead to the development of reconfigurable devices, that can switch efficiently between memory tasks and logic operations. © 2012 Elsevier B.V. All rights reserved.

KEYWORDS: Logic gates; Memory; Nonlinear circuits; Stochastic resonance

http://www.sciencedirect.com/science/article/pii/S0375960112000643

http://dx.doi.org/10.1016/j.physleta.2012.01.039,

181. Parvej Alam., **Maheswararao Karanam.**, **Angshuman Roy Choudhury.,** Inamur Rahaman Laskar **(2012)** *One-pot synthesis of strong solid state emitting mono-cyclometalated iridium(iii) complexes: Study of their aggregation induced enhanced phosphorescence*. **Dalton Transactions, 41 (31), pp. 9276-9279.**

ABSTRACT: Strong solid-state greenish-blue emitting, mono-cyclometalated iridium complexes, [Ir(ppy)(PPh $_{3)}$ $_{2}$(H)(Cl)], 2a and [Ir(F$_2$ppy)(PPh $_{3)}$ $_{2}$(H)(Cl)], 2b [ppyH = 2-phenylpyridine; F$_2$ppyH = 2-(2′,4′-difluoro) phenylpyridine], have been synthesized by a convenient route. The 'aggregation induced enhanced phosphorescence (AIEP)' activity exhibited by these complexes has been rationalized. © 2012 The Royal Society of Chemistry.

KEYWORDS: 2-phenylpyridine; Ir(ppy); Iridium complex; One-pot synthesis, Chlorine compounds; Iridium; Phosphorescence; Synthesis (chemical), Iridium compounds

http://pubs.rsc.org/en/content/articlehtml/2012/dt/c2dt30771e

DOI:10.1039/C2DT30771E

182. S**udesh K. Khanduja.,** Sanjeev Kumar **(2012)** On prolongations of valuations via newton polygons and liftings of polynomials. Journal of Pure and Applied Algebra, 216 (12), 2648-2656.

ABSTRACT : Let v be a real valuation of a field K with valuation ring Rv. Let K(θ) be a finite separable extension of K with θ integral over Rv and F(x) be the minimal polynomial of θ over K. Using Newton polygons and residually transcendental prolongations of v to a simple transcendental extension K(x) of K together with liftings with respect to such prolongations, we describe a method to determine all prolongations of v to K(θ) along with their residual degrees and ramification indices over v. We give an analogue of Ore's Theorem when the base field is an arbitrary rank-1 valued field which extends the main result of [Mathematika, **47** (2000), 173--196].

KEYWORDS: Valued fields; Non-Archimedean valued fields; Irreducible polynomials.

http://www.sciencedirect.com/science/article/pii/S0022404912001223

http://dx.doi.org/10.1016/j.jpaa.2012.03.034,

183. Aitipamula, S., Banerjee, R., Bansal., A.K., Biradha, K., Cheney, M.L., **Angshuman Roy Choudhury.**, Desiraju, G.R., Dikundwar, A.G., Dubey, R., Duggirala, N., Ghogale, P.P., Ghosh, S., Goswami, P.K., Goud, N.R., Jetti, R.K.R., Karpinski, P., Kaushik, P., Kumar, D., Kumar, V., Moulton, B., Mukherjee, A., Mukherjee, G., Myerson, A.S., Puri, V., Ramanan, A., Rajamannar, T., Reddy, C.M., Rodriguez-Hornedo, N., Rogers, R.D., Row, T.N.G., Sanphui, P., Shan, N., Shete, G., Singh, A., Sun, C.C., Swift, J.A., Thaimattam, R., Thakur, T.S., Kumar Thaper, R., Thomas, S.P., Tothadi, S., Vangala, V.R., Vishweshwar, P., Weyna, D.R., Zaworotko, M.J. (2012) *Polymorphs, salts and cocrystals: What's in a name*? ., **Crystal Growth Design.,12(5)pp.2147-2152**

(Erratum : RCrystal Growth and Design, 12 (8), pp. 4290-4291.)

ABSTRACT: the December 2011 release of a draft United States Food and Drug Administration (FDA) guidance concerning regulatory classification of pharmaceutical cocrystals of active pharmaceutical ingredients (APIs) addressed two matters of topical interest to the crystal engineering and pharmaceutical science communities: (1) a proposed definition of cocrystals; (2) a proposed classification of pharmaceutical cocrystals as dissociable “API-excipient” molecular complexes. The Indo–U.S. Bilateral Meeting sponsored by the Indo–U.S. Science and Technology Forum titled *The Evolving Role of Solid State Chemistry in Pharmaceutical Science* was held in Manesar near Delhi, India, from February 2–4, 2012. A session of the meeting was devoted to discussion of the FDA guidance draft. The debate generated strong consensus on the need to define cocrystals more broadly and to classify them like salts. It was also concluded that the diversity of API crystal forms makes it difficult to classify solid forms into three categories that are mutually exclusive. This perspective summarizes the discussion in the Indo–U.S. Bilateral Meeting and includes contributions from researchers who were not participants in the meeting.

http://pubs.acs.org/doi/abs/10.1021/cg3002948

DOI: 10.1021/cg3002948

184. Akhilesh Kumar., **Anand K. Bachhawat (2012)** *Pyroglutamic acid: Throwing light on a lightly studied metabolite.* **Current Science, 102 (2), pp. 288-297.**

ABSTRACT: Pyroglutamic acid or 5-oxoproline is the cyclic lactam of glutamic acid. Its presence in living cells has been reported from archaebacteria to humans, and its occurrence in living cells has been known for over a century. Despite its almost ubiquitous presence, the role of pyroglutamic acid in living cells is poorly understood. Pyroglutamic acid is found as an N-terminal modification in many neuronal peptides and hormones that also include the accumulating peptides in Alzheimer's disease and familial dementia. The modification is also observed in proteins that include many antibodies, some enzymes and structural proteins. The modification in proteins has been shown to contribute to both the structural and activity-related properties of the proteins. Pyroglutamate also exists as a free metabolite in living cells. In several genetic disorders of humans, and in an acetaminophen-induced metabolic disorder, high levels of pyroglutamic acid are secreted in the urine in what is known as 5-oxoprolinuria. The proposed functions of free pyroglutamic acid include its role as an analogue or reservoir of glutamate, as well as other functions unique to it, that includes a possible role in osmoprotection. This short review tries to capture our current understanding of pyroglutamic acid in living cells.

KEYWORDS: γ-Glutamyl cycle; 5-oxoproline; 5-oxoprolinuria; Neuronal peptides; Pyroglutamic acid

www.currentscience.ac.in/cs/Volumes/102/02/0288.pdf

185. M.Majumder., **N.Sathyamurthy.,** H.Lefebvre-Brion., G.J.Vázquez **(2012)** *Photoabsorption of carbon monoxide: A time-dependent quantum mechanical study.* **Journal of Physics B: Atomic, Molecular and Optical Physics, 45 (18), art. no. 185101.**

ABSTRACT: Photoabsorption cross-section values are computed for the $A^1\Pi$–$X^1\Sigma$ transition in $^{12}C^{16}O$ by a time-dependent quantum mechanical method. The computed oscillator strength values are shown to be in good agreement with the available experimental and theoretical values. The small differences between our computed oscillator strength values and the experimental results could be accounted for by the weak interactions between the $A^1\Pi$ state and triplet states ($a^3\Sigma+$,$e^3\Sigma-$and$d^3\Delta$) that cross the PEC of the A state near its minimum. Calculations for different isotopologues of CO(12C 17O, 12C 18O and 13C 16O) reveal a mass dependence that becomes more significant for higher vibrational levels. © 2012 IOP Publishing Ltd.

KEYWORDS: Cross-section values; Isotopologues; Oscillator strengths; Photoabsorptions; Quantum mechanical method; Quantum-mechanical study; Theoretical values; Time-dependent; Triplet state; Vibrational levels; Weak interactions, Carbon monoxide; Radiation, Quantum theory

http://iopscience.iop.org/0953-4075/45/18/185101/article

Doi:10.1088/0953-4075/45/18/185101

186. Preety Aneja., Ramandeep S. Johal (2012) *Prior probabilities and thermal characteristics of heat engines* . **Central European Journal of Physics, 10 (3), pp. 708-714.**

ABSTRACT: The thermal characteristics of a heat cycle are studied from a Bayesian approach. In this approach, we assign a certain prior probability distribution to an uncertain parameter of the system. Based on that prior, we study the expected behaviour of the system and it has been found that even in the absence of complete information, we obtain thermodynamic-like behaviour of the system. Two models of heat cycles, the quantum Otto cycle and the classical Otto cycle are studied from this perspective. Various expressions for thermal efficiences can be obtained with a generalised prior of the form Π(x) ∝ 1/x b. The predicted thermodynamic behaviour suggests a connection between prior information about the system and thermodynamic features of the system. © 2012 Versita Warsaw and Springer-Verlag Wien.

KEYWORDS: Otto cycle; prior information; quantum heat engines; subjective probability

http://link.springer.com/article/10.2478%2Fs11534-012-0042-y?LI=true#page-1

DOI: 10.2478/s11534-012-0042-y

187. Gurmeet K. Bakshi., **Inder Bir S. Passi (2012)** *Primitive Central Idempotents in Rational Group Algebras* . **Communications in Algebra, 40 (4), pp. 1413-1426.**

ABSTRACT: A complex irreducible character χ of a finite group G, with an affording representation ρ, is defined to have the property P if, for all g ∈ G, either χ(g) = 0 or all the eigen-values of ρ(g) have the same order. An explicit expression for the primitive central idempotent of the rational group algebra Q [G] associated with a complex irreducible character having the property P is derived. Several consequences are then obtained. © 2012 Copyright Taylor and Francis Group, LLC.

KEYWORDS: Irreducible complex representation; Primitive central idempotent; Rational group algebra; Wedderburn decomposition

http://www.tandfonline.com/doi/abs/10.1080/00927872.2010.551685

DOI:10.1080/00927872.2010.551685

188. P.Mandal., A.Nandi., **S. Anantha Ramakrishna (2012)** *Propagating surface plasmon resonances in two-dimensional patterned gold-grating templates and surface enhanced Raman scattering*. **Journal of Applied Physics, 112 (4), art. no. 044314.**

ABSTRACT: Surface enhanced Raman scattering (SERS) from Raman active rhodamine-6G probe molecules is investigated on two-dimensional patterned gold-grating templates having submicron periodicity of 800 nm. Two-dimensional surface nano-patterning in the form of square, hexagonal, and rectangle has been obtained through cost effective laser interference lithography. We find a reproducible SERS enhancement of the order of 10 5 on these nano-patterned plasmonic templates, showing a slight superior result on hexagonal patterned templates. Strong localized near-fields due to surface plasmon resonance (SPR) lead to such an enhancement. We find evidence for good correlation in the SPR excitation and enhanced Raman scattering through experimental investigation by using different Raman pump excitation wavelengths of 785 nm, 633 nm, and 514 nm and different pump powers. The results are strongly supported by computer simulations of the electromagnetic fields at the pump wavelengths. Our results demonstrate that an optimized selection of the structure and pump excitation wavelength is necessary for good SERS signal. © 2012 American Institute of Physics.

KEYWORDS: Cost effective; Enhanced Raman scattering; Experimental investigations; Good correlations; Laser interference lithography; NanoPatterning; Optimized selection; Plasmonic; Probe molecules; Pump excitation; Pump power; Pump wavelength; Raman pump; Rhodamine 6G; SERS enhancement; SPR excitation; Submicron; Surface enhanced Raman Scattering (SERS); Two-dimensional surface, Electromagnetic fields; Gold; Pumps; Raman scattering; Raman spectroscopy; Surface plasmon resonance, Two dimensional

http://jap.aip.org/resource/1/japiau/v112/i4/p044314_s1

http://dx.doi.org/10.1063/1.4748180

189. Saurabh Srivastava., **N. Sathyamurthy (2012)** *Radiative lifetimes of spin forbidden $a^1\Delta \rightarrow X\ ^3\Sigma^-$ and spin allowed $A^3\Pi \rightarrow X\ ^3\Sigma$- transitions and complete basis set extrapolated ab initio potential energy curves for the ground and excited states of CH^-* Journal of Chemical Physics, 137 (21), art. no. 214314, .

ABSTRACT: The spin forbidden transition $a^1\Delta \rightarrow X\ ^3\Sigma$- in CH^- has been studied using the Breit-Pauli Hamiltonian for a large number of geometries. This transition acquires intensity through spin-orbit coupling with singlet and triplet Π states. The transition moment matrix including more than one singlet and triplet Π states was calculated at the multi-reference configuration interaction/aug-cc-pV6Z level of theory. The computed radiative lifetime of 5.63 s is in good agreement with the experimental (5.9 s) and other theoretical (6.14 s) results. Transition moment values of the spin allowed $A^3\Pi \rightarrow X^3\Sigma$- transition have also been calculated at the same level of theory. Calculations show that the corresponding radiative lifetime is considerably low, 2.4×10^{-7} s. Complete basis set extrapolated potential energy curves for the ground state of CH and the ground state and six low lying excited states ($a^1\Delta$, $b^1\Sigma^{+,}$ two $^3\Pi$, and two $^1\Pi$) of CH^- are reported. These curves are then used to calculate the vibrational bound states for CH and CH^-. The computed electron affinity of CH supports the electron affinity bounds reported by Okumura [J. Chem. Phys. 85, 1971 (1986)10.1063/1.451140]. © 2012 American Institute of Physics.

KEYWORDS: Ab initio potential energy curves; Bound state; Complete basis sets; Forbidden transitions; Low-lying excited state; Multireference configuration; Potential energy curves; Radiative lifetime; Spin-orbit couplings; Transition moments, Calculations; Excited states; Extrapolation; Ground state; Potential energy, Nuclear physics

http://jcp.aip.org/resource/1/jcpsa6/v137/i21/p214314_s1

http://dx.doi.org/10.1063/1.4768873

190 Junaid Khan., Shelly Gupta, Kausik Chattopadhyay., Arunika Mukhopadhaya (2012) *Refolding and functional assembly of the Vibrio cholerae porin OmpU recombinantly expressed in the cytoplasm of Escherichia coli*. **Protein Expression and Purification, 85 (2), 204-210.**

ABSTRACT: OmpU is one of the major outer membrane porins of *Vibrio cholerae*. OmpU has been biochemically characterized previously for its 'porin'-property. However, previous studies have used the OmpU protein extracted from the bacterial outer membrane envelope fractions. Such method of isolation imposes limitations on the availability of the protein reagent, and also enhances the possibility of the OmpU preparation being contaminated with lipid molecules of bacterial outer membrane origin, especially lipopolysaccharides (LPS). Here we report a strategy of purifying the *V. cholerae* OmpU protein recombinantly overexpressed in heterologous protein expression system in *Escherichia coli*, without its being incorporated into the bacterial membrane fraction. In our strategy, the majority of the protein was expressed as insoluble inclusion body in the *E. coli* cytoplasm, the protein was dissolved by denaturation in 8 M urea, refolded, and purified to homogeneity in presence of detergent. Our strategy allowed isolation of the recombinant OmpU protein with significantly enhanced yield as compared to that of the wild type protein extracted from the *V. cholerae* membrane fraction. The recombinant *V. cholerae* OmpU protein generated in our study displayed functional channel-forming property in the synthetic liposome membrane, thus confirming its 'porin'-property. To the best of our knowledge, this is the first report showing an efficient refolding and functional assembly of the *V. cholerae* OmpU porin recombinantly expressed as inclusion body in the cytoplasm of a heterologous host *E. coli*.

Keywords: Porin, OmpU, *Vibrio cholerae*, Membrane protein, Refolding

http://www.sciencedirect.com/science/article/pii/S1046592812002148
http://dx.doi.org/10.1016/j.pep.2012.08.005,

191. Yogesh Singh., S. Manni, J. Reuther., T. Berlijn. R. Thomale., W. Ku, S. Trebst., P. Gegenwart (**2012**) *Relevance of the Heisenberg-Kitaev model for the honeycomb lattice iridates A_2IrO_3* **Physical Review Letters, 108 (12), art. no. 127203,** .

ABSTRACT: Combining thermodynamic measurements with theoretical calculations we demonstrate that the iridates A_2IrO_3 (A=Na, Li) are magnetically ordered Mott insulators where the magnetism of the effective spin-orbital S=1/2 moments can be captured by a Heisenberg-Kitaev (HK) model with interactions beyond nearest-neighbor exchange. Experimentally, we observe an increase of the Curie-Weiss temperature from θ-125K for Na_2IrO_3 to θ-33K for Li_2IrO_3, while the ordering temperature remains roughly the same $T_N \approx$ 15K. Using functional renormalization group calculations we show that this evolution of θ and T_N as well as the low temperature zigzag magnetic order can be captured within this extended HK model. We estimate that Na_2IrO_3 is deep in a magnetically ordered regime, while Li_2IrO_3 appears to be close to a spin-liquid regime. © 2012 American Physical Society.

KEYWORDS: Curie-Weiss temperature; Functional renormalization group; Honeycomb lattices; Low temperatures; Magnetic orders; Mott insulators; Nearest-neighbors; Ordering temperature; Spin-liquid; Spin-orbitals; Theoretical calculations; Thermodynamic measurements, Sodium; Statistical mechanics, Ion exchange

http://prl.aps.org/abstract/PRL/v108/i12/e127203

http://arxiv.org/abs/1106.0429

DOI:10.1103/PhysRevLett.108.127203

192. Kamal P. Singh., Rajeev Kapri., Sudeshna Sinha (2012) *Scalable ultra-sensitive detection of heterogeneity via coupled bistable dynamics* . **Europhysics Letters, 98 (6), art. no. 60004,** .

ABSTRACT: We demonstrate how the collective response of N globally coupled bistable elements can strongly reflect the presence of very few non-identical elements in a large network of otherwise identical elements. Counter-intuitively, when there are a small number of elements with natural stable state different from the bulk of the elements, all the elements of the system evolve to the stable state of the minority due to strong coupling. The critical fraction of distinct elements needed to produce this swing shows a sharp transition with increasing N, scaling as . Furthermore, one can find a global bias that allows robust one-bit sensitivity to heterogeneity. Importantly, the time needed to reach the attracting state does not increase with the system size. We indicate the relevance of this ultra-sensitive generic phenomenon for massively parallelized applications, such as the determination of the existence of a needle in a haystack by one measurement. © 2012 EPLA.

iopscience.iop.org/0295-5075/98/6/.../0295-5075_98_6_60004.pdf

http://dx.doi.org/10.1209/0295-5075/98/60004
doi:10.1209/0295-5075/98/60004

193. H.K.Jassal (2012) *Scalar field dark energy perturbations and the integrated Sachs-Wolfe effect* . **Physical Review D - Particles, Fields, Gravitation and Cosmology, 86 (4), art. no. 043528,** .

ABSTRACT: Dark energy perturbation affects the growth of matter perturbations even in scenarios with noninteracting dark energy. We investigate the integrated Sachs-Wolfe effect in various canonical scalar field models with perturbed dark energy. We do this analysis for models belonging to the thawing and freezing classes, which are classes based on the way the equation of state evolves with time. For thawing models, the dark energy equation of state remains the same as that of a cosmological constant and deviates from this value at late times. In freezing models, the equation of state evolves in the opposite manner, namely it "freezes" to cosmological constant-type behavior at late times. We show that between these classes there is no clear difference for the Sachs-Wolfe effect. We show that on taking perturbations into account, the contribution due to different models is closer to each other and to the cosmological constant model than it is to the case of an unperturbed scalar field, i.e., the dark energy component is homogeneous. Therefore, considering dark energy to be homogeneous gives an overestimate in distinction between different models.

However, the difference between contribution to the angular power spectrum due to different models remains large, and future observations pertaining to growth of perturbations may be able to distinguish between these. © 2012 American Physical Society.

http://prd.aps.org/abstract/PRD/v86/i4/e043528

DOI:10.1103/PhysRevD.86.043528

194. Vandana Thaplyal., **Sanjeev Sharma.**, Ajay Ballabh Bhatt (**2012**) *Sacred groves as ethnobotanical gene pools in tribal areas of the western Himalayas in India: case study of Kinnaur district in Himachal Pradesh,* **The Indian Forester. Vol. 138 (1) pp.,70-83 .**

ABSTRACT: Study of sacred groves of Kinnaur district, based on the field survey, using GPS, topo sheets and village maps, supported with questionnaire survey in 17 sacred groves revealed the presence of 96 plant species of ethnobotanical importance within 77 genera and 41 families, representing 10 gymnosperms and 86 angiosperms. The species distributed as 22 trees, 32 shrubs and 42 herbs. As per the IUCN standards, 15 species are endangered, 17 are vulnerable and 6 are critically endangere

KEYWORDS: Sacred Groves, Biodiversity, Communities, Conservation, Ethnobotanical Importance

http://www.indianforester.co.in/index.php/indianforester/article/view/4564

195. Karan Paul., Kausik Chattopadhyay (2012) *Single point mutation in Vibrio cholerae cytolysin compromises membrane pore-formation mechanism of the toxin*. **FEBS Journal, 279 (21), 4039- 4051.**

ABSTRACT *: Vibrio cholerae* cytolysin (VCC) belongs to the family of β-barrel pore-forming protein toxins. VCC is secreted by the bacteria as water-soluble monomers, which upon binding to target eukaryotic cells form transmembrane heptameric β-barrel channels. High-resolution 3D structures are described both for the water-soluble monomeric form and the transmembrane oligomeric pore; albeit that our understanding of the mechanistic details of the membrane pore-

formation process remains incomplete. Here, we report the characterization of a nonfunctional VCC variant harboring a single point mutation of Ala425Val positioned within a potential membrane-interacting loop in the VCC structure. The mutation appears to affect interaction of the toxin with erythrocytes as well as cholesterol-containing liposome membrane, without affecting the oligomerization ability of the membrane-bound toxin molecules. The membrane-bound oligomers formed by this VCC mutant do not appear to represent the functional pore assembly of the toxin; rather, such assembly could be considered as being trapped in an abortive, nonfunctional oligomeric state. Our results suggest that the Ala425Val mutation in VCC critically compromises its cholesterol-dependent membrane-interaction mechanism and also abrogates the process of functional membrane pore formation by the toxin.

KEYWORDS : Bacterial protein toxin, cholesterol, membrane, pore-forming toxin, *Vibrio cholerae* cytolysin

http://onlinelibrary.wiley.com/doi/10.1111/j.1742-4658.2012.08809.x/abstract
DOI: 10.1111/j.1742-4658.2012.08809.x

196. S.K.Choi., R.Coldea., A.N.Kolmogorov., T.Lancaster., I.I.Mazin., S.J.Blundell., P.G.Radaelli., **Yogesh Singh.**, P.Gegenwart., K.R.Choi., S.-W.Cheong., P.J.Baker, C.Stock., J.Taylor (**2012**) *Spin waves and revised crystal structure of honeycomb iridate* Na_2IrO_3 *.* **Physical Review Letters, 108 (12), art. no. 127204, .**

ABSTRACT: We report inelastic neutron scattering measurements on Na 2IrO 3, a candidate for the Kitaev spin model on the honeycomb lattice. We observe spin-wave excitations below 5meV with a dispersion that can be accounted for by including substantial further-neighbor exchanges that stabilize zigzag magnetic order. The onset of long-range magnetic order below T N=15.3K is confirmed via the observation of oscillations in zero-field muon-spin rotation experiments. Combining single-crystal diffraction and density functional calculations we propose a revised crystal structure model with significant departures from the ideal 90°Ir-O-Ir bonds required for dominant Kitaev exchange. © 2012 American Physical Society.

KEYWORDS: Honeycomb lattices; Inelastic neutrons; Long range magnetic order; Magnetic orders; Muon spin rotation; Single-crystal diffraction; Spin models; Spinwave excitation; Zero fields, Density functional theory; Honeycomb structures; Iridium; Sodium, Spin waves

http://prl.aps.org/abstract/PRL/v108/i12/e127204

DOI:10.1103/PhysRevLett.108.127204

197. S. Sharma (2012) *Strategies for technical sustainable development of hydropower projects in the mountain environment by adopting participatory approach.* **Indian Journal of Power and River Valley Development. 61 (9&10): 147-153 .**

ABSTRACT *: T*o meet the ever growing demand for energy around the world, we need more sophisticated technology for the development of hydropower projects in the mountain environment so that the frazile environment is not adversely affected. While for suggesting measures to minimise the adverse impacts the need of the local community participation should also be considered. Increasing environmental awareness in a time phase manner under traditional practices to stabilize hill slopes is important. Preparing the public to face hazardous situations and capacity building is must. This would promote hydropower development which can be accepted by the affected people, society, hydropower authority, government and non-governmental organisations.

http://www.connectjournals.com/subscription_info.php?bookmark=CJ-001162

198. Gurpreet Kaur., Piyush Panini., Deepak Chopra.**, Angshuman Roy Choudhury (2012)** *Structural investigation of weak intermolecular interactions in fluorine substituted isomeric N-benzylideneanilines* . **Crystal Growth and Design, 12 (10), pp. 5096-5110.**

ABSTRACT: The study of the influence of aromatic C-F group in directing crystal packing is an important area of current research. The role of the aromatic

C-F group in the formation of weak intermolecular interactions in the absence of strong hydrogen bond donors and acceptors has been analyzed in a series of 15 newly synthesized fluorine substituted (mono- and di-) isomeric N-benzylideneanilines. It was observed that five compounds (out of a total number of 15) were liquids at room temperature, while others have low melting points (<60 °C). In situ crystallization, using an optical heating and crystallization device (OHCD), has been used to crystallize and determine the crystal structures of three out of five compounds which were found to be liquids at 25 °C. A detailed investigation of the molecular conformation and the crystal packing in these compounds reveals that the presence of organic fluorine acts as a significant contributor in the construction of various supramolecular synthons, essentially using a variety of C-H···F intermolecular interactions. These have been found to generate different three-dimensional arrangements of molecules in the crystalline framework. In order to realize the stabilizing influence exerted by such weak interactions, intermolecular C-H···F interaction energies have been calculated using Firefly to quantify the strength of such interactions. Lattice energy calculations have been performed and the individual energies, namely, the Coulombic, polarization, dispersion, and repulsive contributions to the lattice energy have been determined using the CLP program. In addition to these, theoretical calculations have been performed at the density functional theory level, and the experimental geometry has been compared with the optimized geometry to highlight the importance of molecular conformation in the solid and gas phase. It is of interest to note that stabilization resulting from the presence of C-H···F interactions, albeit less, is not negligible and does contribute toward crystal packing. © 2012 American Chemical Society.

KEYWORDS: CLP programs; Crystal packings; Gasphase; Hydrogen bond donors; In-situ crystallization; Interaction energies; Intermolecular interactions; Lattice energies; Lattice energy calculations; Low melting point; Molecular conformation; N-benzylideneanilines; Optical heating; Optimized geometries; Organic fluorine; Room temperature; Structural investigation; Supramolecular synthons; Theoretical calculations; Weak interactions, Aromatic compounds; Conformations; Density functional theory, Fluorine

http://pubs.acs.org/doi/abs/10.1021/cg3010294

DOI:10.1021/cg3010294

199. Mily Bhattacharya., Samrat Mukhopadhyay (2012) *Structural and dynamical insights into the molten-globule form of ovalbumin*. **Journal of Physical Chemistry B, 116 (1), pp. 520-531.**

ABSTRACT: Ovalbumin is a 45 kDa egg-white glycoprotein which belongs to the class of serpin superfamily. We have studied the structural properties of both native and partially unfolded molten-globule forms of ovalbumin using a diverse array of spectroscopic tools. Time-resolved fluorescence measurements provided important structural and dynamical insights into the native and molten-globule states. Fluorescence anisotropy decay analysis indicated that there is a conformational swelling from the native to the molten-globule form of ovalbumin. We have also carried out red-edge excitation shift measurements to probe the dipolar relaxation dynamics around the intrinsic tryptophan residues. Additionally, stopped-flow fluorescence experiments revealed that the conformational transition from the native to the molten-globule form proceeds in a stepwise manner involving a burst-phase with a submillisecond conformational change followed by biphasic slower conformational reorganizations on the millisecond time scale leading to the final molten-globule state. © 2011 American Chemical Society.

KEYWORDS: Biphasic; Conformational change; Conformational transitions; Dipolar relaxation; Excitation shift; Fluorescence anisotropy decay; Intrinsic tryptophans; Ovalbumins; Spectroscopic tool; Stopped flow; Time-resolved fluorescence measurements; Time-scales, Amino acids, Fluorescence, ovalbumin, article; chemistry; circular dichroism; kinetics; pH; protein denaturation; protein secondary structure; protein tertiary structure; spectrofluorometry, Circular Dichroism; Hydrogen-Ion Concentration; Kinetics; Ovalbumin; Protein Denaturation; Protein Structure, Secondary; Protein Structure, Tertiary; Spectrometry, Fluorescence

http://pubs.acs.org/doi/abs/10.1021/jp208416d

DOI: 10.1021/jp208416d

200. Harris, E. J., **Sinha, B.**, Foley, S., Crowley, J. N., Borrmann, S., Hoppe P. (**2012**) *Sulfur isotope fractionation during heterogeneous oxidation of SO_2 by mineral dust.* Atmospheric Chemistry and Physics, 12, pp.,4867-4884.

ABSTRACT: Mineral dust is a major fraction of global atmospheric aerosol, and the oxidation of SO_2 on mineral dust has implications for cloud formation, climate and the sulfur cycle. Stable sulfur isotopes can be used to understand the different oxidation processes occurring on mineral dust. This study presents measurements of the $^{34}S/^{32}S$ fractionation factor α_{34} for oxidation of SO_2 on mineral dust surfaces and in the aqueous phase in mineral dust leachate. Sahara dust, which accounts for ~60% of global dust emissions and loading, was used for the experiments. The fractionation factor for aqueous oxidation in dust leachate is $\alpha_{leachate} = 0.9917\pm0.0046$, which is in agreement with previous measurements of aqueous SO_2 oxidation by iron solutions. This fractionation factor is representative of a radical chain reaction oxidation pathway initiated by transition metal ions. Oxidation on the dust surface at subsaturated relative humidity (RH) had an overall fractionation factor of $\alpha_{het} = 1.0096\pm0.0036$ and was found to be almost an order of magnitude faster when the dust was simultaneously exposed to ozone, light and RH of ~40 %. However, the presence of ozone, light and humidity did not influence isotope fractionation during oxidation on dust surfaces at subsaturated relative humidity. All the investigated reactions showed mass-dependent fractionation of ^{33}S relative to ^{34}S. A positive matrix factorization model was used to investigate surface oxidation on the different components of dust. Ilmenite, rutile and iron oxide were found to be the most reactive components, accounting for 85% of sulfate production with a fractionation factor of $\alpha_{34} = 1.012\pm0.010$. This overlaps within the analytical uncertainty with the fractionation of other major atmospheric oxidation pathways such as the oxidation of SO_2 by H_2O_2 and O_3 in the aqueous phase and OH in the gas phase. Clay minerals accounted for roughly 12% of the sulfate production, and oxidation on clay minerals resulted in a very distinct fractionation factor of $\alpha_{34} = 1.085\pm0.013$. The fractionation factors measured in this study will be particularly useful in combination with field and modelling studies to understand the role of surface oxidation on clay minerals and aqueous oxidation by mineral dust and its leachate in global and regional sulfur cycles.

KEYWORDS : aerosol iron solubility; saharan dust; nitric-acid; photocatalytic oxidation; tropospheric chemistry; anthropogenic sources; gas desulfurization; atmospheric sulfate; gaseous pollutants; calcium-*carbonate*

http://www.atmos-chem-phys.net/12/4867/2012/acp-12-4867-2012.pdf

doi:10.5194/acp-12-4867-2012

201.. E.Harris., **B.Sinha.,** P.Hoppe, J.N., Crowley., S.Ono., S.Foley (**2012**) *Sulfur isotope fractionation during oxidation of sulfur dioxide: gas-phase oxidation by OH radicals and aqueous oxidation by H_2O_2,O_3 and iron catalysis.* **Atmos. Chem. Phys., 12, 407-423, 2012**

ABSTRACT: The oxidation of SO_2 to sulfate is a key reaction in determining the role of sulfate in the environment through its effect on aerosol size distribution and composition. Sulfur isotope analysis has been used to investigate sources and chemical processes of sulfur dioxide and sulfate in the atmosphere, however interpretation of measured sulfur isotope ratios is challenging due to a lack of reliable information on the isotopic fractionation involved in major transformation pathways. This paper presents laboratory measurements of the fractionation factors for the major atmospheric oxidation reactions for SO_2: Gas-phase oxidation by OH radicals, and aqueous oxidation by H_2O_2, O_3 and a radical chain reaction initiated by iron. The measured fractionation factor for $^{34}S/^{32}S$ during the gas-phase reaction is $\alpha_{OH} = (1.0089\pm0.0007)-((4\pm5)\times10^{-5})$ T(°C). The measured fractionation factor for $^{34}S/^{32}S$ during aqueous oxidation by H_2O_2 or O_3 is $\alpha_{aq} = (1.0167\pm0.0019)-((8.7\pm3.5)\times10^{-5})T$(°C). The observed fractionation during oxidation by H_2O_2 and O_3 appeared to be controlled primarily by protonation and acid-base equilibria of S(IV) in solution, which is the reason that there is no significant difference between the fractionation produced by the two oxidants within the experimental error. The isotopic fractionation factor from a radical chain reaction in solution catalysed by iron is $\alpha_{Fe} = (0.9894\pm0.0043)$ at 19 °C for $^{34}S/^{32}S$. Fractionation was mass-dependent with regards to $^{33}S/^{32}S$ for all the reactions investigated. The radical chain reaction mechanism was the only measured reaction that had a faster rate for the light isotopes. The results presented in this study will be particularly useful to determine the importance of the transition metal-catalysed oxidation pathway compared to other oxidation pathways, but other main oxidation pathways can not be distinguished based on stable sulfur isotope measurements alone.

http://www.atmos-chem-phys.net/12/407/2012/acp-12-407-2012.html

doi:10.5194/acp-12-407-2012

202. A.C.Nölscher., J.Williams., **V.Sinha.**, T.Custer., W.Song., A.M.Johnson., R.Axinte., H.Bozem., H.Fischer., N.Pouvesle., G.Phillips., J.N.Crowley., P.Rantala., J.Rinne., M.Kulmala., D.Gonzales., J.Valverde-Canossa., A.Vogel, T.Hoffmann., H.G.Ouwersloot., J.Vilà-Guerau De Arellano., J.Lelieveld. **(2012**) *Summertime total OH reactivity measurements from boreal forest during HUMPPA-COPEC 2010.* Atmospheric **Chemistry and Physics, 12 , pp. 7419–7452**

ABSTRACT: Ambient total OH reactivity was measured at the Finnish boreal forest station SMEAR II in Hyytiälä (Latitude 61°51' N; Longitude 24°17' E) in July and August 2010 using the Comparative Reactivity Method (CRM). The CRM - total OH reactivity method - is a direct, in-situ determination of the total loss rate of hydroxyl radicals (OH) caused by all reactive species in air. During the intensive field campaign HUMPPA-COPEC 2010 (Hyytiälä United Measurements of Photochemistry and Particles in Air - Comprehensive Organic Precursor Emission and Concentration study) the total OH reactivity was monitored both inside (18 m) and directly above the forest canopy (24 m) for the first time. The comparison between these two total OH reactivity measurements, absolute values and the temporal variation have been analyzed here. Stable boundary layer conditions during night and turbulent mixing in the daytime induced low and high short-term variability, respectively. The impact on total OH reactivity from biogenic emissions and associated photochemical products was measured under "normal" and "stressed" (i.e. prolonged high temperature) conditions. The advection of biomass burning emissions to the site caused a marked change in the total OH reactivity vertical profile. By comparing the OH reactivity contribution from individually measured compounds and the directly measured total OH reactivity, the size of any unaccounted for or "missing" sink can be deduced for various atmospheric influences. For "normal" boreal conditions a missing OH reactivity of 58%, whereas for "stressed" boreal conditions a missing OH reactivity of 89% was determined. Various sources of not quantified OH reactive species are proposed as possible explanation for the high missing OH reactivity.

KEYWORDS: advection; ambient air; biogenic emission; biomass burning; boreal forest; boundary layer; forest canopy; hydroxyl radical; *photochemistry; temporal variation*

www.atmos-chem-phys-discuss.net/12/7419/2012 /

doi:10.5194/acpd-12-7419-2012

203. Sadhika Khullar. , Sanjay K. Mandal (2012) *Supramolecular assemblies of dimanganese subunits and water clusters organized by strong hydrogen bonding interactions: Single crystal to single crystal transformation by thermal De-/rehydration processes.* **Crystal Growth and Design, 12 (11), pp. 5329-5337.**

ABSTRACT: New three-dimensional (3D) supramolecular assemblies held together by strong hydrogen bonding interactions between two-dimensional (2D) layers of the $[Mn_2(adc)_2(bpta)_2(H_2O)_2]$ subunit (where adc = acetylene dicarboxylate and bpta = N,N-bis-(2- pyridylmethyl)-tert-butylamine) containing a pore (8.225 Å × 4.048 Å) and a cluster of water molecules (five at 296 K and six at 120 K) are reported. The water cluster arrangement in the channel is found to be different at these two temperatures. In the two-dimensional layers, there exists strong intermolecular hydrogen bonding interactions (O···H-O) between the uncoordinated oxygen atoms of the adc and hydrogen atoms of the bound water molecules. $[Mn_2(adc)_2(bpta)_2(H_2O)_2]\cdot 5H_2O$ ($1\cdot 5H_2O$) is prepared by mixing equimolar amounts of bpta and $Mn(ClO_4)_2\cdot 6H_2O$ in methanol at room temperature followed by the addition of 1 equiv of disodium acetylene dicarboxylate in 55% yield. Direct layering of the starting materials results in the formation of a similar 3D supramolecular assembly, $1\cdot 4H_2O\cdot CH_3OH$. When a single crystal of $1\cdot 5H_2O$ is slowly heated to 350 K, it undergoes a solid-state structural transformation to the 2D framework 1, where the cluster of five water molecules in the channel of the former is completely removed, showing remarkable stability. Upon rehydration of 1 under ambient conditions over a few weeks, the 3D supramolecular assembly $1\cdot 4H_2O$, where strong hydrogen bonding as well as C-H···O interactions exist, was obtained. The solid-state structural transformation between 3D, 2D, and 3D during the dehydration and rehydration processes in $1\cdot 5H_2O$, 1, and $1\cdot 4H_2O$, respectively, was verified by single crystal and powder XRD measurements. These compounds were also characterized by elemental analysis, IR, and Raman spectroscopy and thermogravimetric and differential scanning calorimetry analyses. © 2012 American Chemical Society.

KEYWORDS: Ambient conditions; Bound water molecules; Equimolar amount; Hydrogen atoms; Hydrogen bonding interactions; Intermolecular hydrogen bonding; Oxygen atom; Rehydration process; Room temperature; Single crystal-to-single-crystal transformation; Single-crystal and powder; Structural transformation; Supramolecular assemblies; Thermogravimetric; Water cluster; Water molecule, Acetylene; Azobenzene; Carboxylation; Differential scanning calorimetry; Hydrogen bonds; Lighting; Manganese; Methanol; Molecules; Raman spectroscopy; Single crystals; Three dimensional computer graphics; Two dimensional, Manganese compounds

http://pubs.acs.org/doi/abs/10.1021/cg300937f

DOI: 10.1021/cg300937f

204. Venderbos., J.W.F., Daghofer., M., Van Den Brink, J., **Kumar, S. (2012)** *Switchable quantum anomalous hall state in a strongly frustrated lattice magnet.* Physical Review Letters, 109 (16), art. no. 166405, .

ABSTRACT: We establish that the interplay of itinerant fermions with localized magnetic moments on a checkerboard lattice leads to magnetic flux phases. For weak itineracy the flux phase is coplanar and the electronic dispersion takes the shape of graphenelike Dirac fermions. Stronger itineracy drives the formation of a noncoplanar, chiral flux phase, in which the Dirac fermions acquire a topological mass that is proportional to a ferromagnetic spin polarization. Consequently the system self-organizes into a ferromagnetic quantum anomalous Hall state in which the direction of its dissipationless edge currents can be switched by an applied magnetic field. © 2012 American Physical Society.

KEYWORDS: Applied magnetic fields; Dirac fermions; Edge currents; Electronic dispersions; Ferromagnetic spin; Flux phase; Hall state; Localized magnetic moments; Non-coplanar; Switchable, Ferromagnetic materials; Ferromagnetism; Magnetic flux; Magnetic moments, Quantum theory

http://arxiv.org/abs/1202.3340

http://prl.aps.org/abstract/PRL/v109/i16/e166405

DOI:10.1103/PhysRevLett.109.166405

205. Prashanth, B., Karanam, M., Choudhury, A.R., Singh, S.(**2012**) *Synthesis, spectroscopic and structural characterization of Co(II), Ni(II) and Cu(II) complexes of substituted 2-pyridyl amine based [N,N] chelating ligand*. **Polyhedron, 47 (1), pp. 112-117.**

ABSTRACT: The reaction of N-benzylaminopyridine with the imidoylchloride of N-(2,6-$_i$Pr$_2$C$_6$H$_3$)acetamide in the presence of Et_3N affords a new neutral [N,N] chelating ligand, (PhCH$_2$)N(2-pyridyl)C{(Me)(N-2,6-$_i$Pr$_2$C$_6$H$_3$)} (L). The reaction of equimolar quantities of L with $Cu(NO_3)_2$, $CuCl_2$ and $NiBr_2$, respectively, in DCM, acetonitrile and DME yields the corresponding mononuclear complexes $L\cdot Cu(NO_3)_2$ (1), $L\cdot CuCl_2$ (2) and $L\cdot NiBr_2$ (3). Whereas, the reaction of L with $CoCl_2\cdot 6H_2O$ leads to the formation of $[HL\cdot CoCl_3]$ (4) with pyridine nitrogen coordinated to cobalt. Solid state structure of L and compounds 1-4 have been investigated by single crystal X-ray structural analysis. The ligand L shows the E-anti arrangement in the solid state and its mononuclear complex 1 shows six coordinated Cu in a quasi square planar geometry with two long distanced donors; complexes 2 and 3 show distorted tetrahedral arrangement of the substituents around metal ions. Interestingly, the solid state structure of complex 4 reveals C-H···Cl intra-molecular hydrogen bonding and N-H···Cl and C-H···Cl inter-molecular hydrogen bonds. These hydrogen bonding interactions in complex 4 facilitate the formation of an extended 2D network structure. © 2012 Elsevier Ltd. All rights reserved.

KEYWORDS: Cobalt complex; Copper complex; Hydrogen bonding; Pyridyl amine; Tetrahedral nickel complex

http://www.sciencedirect.com/science/article/pii/S0277538712005931

http://dx.doi.org/10.1016/j.poly.2012.08.019

206. Nölscher, A.C., **Sinha, V.**, Bockisch, S., Klüpfel, T., Williams, J. (**2012**) *Total OH reactivity measurements using a new fast gas chromatographic photo-ionization detector (GC-PID*) Atmospheric Measurement Techniques, 5 (12), pp. 2981-2992.

ABSTRACT: The primary and most important oxidant in the atmosphere is the hydroxyl radical (OH). Currently OH sinks, particularly gas phase reactions, are poorly constrained. One way to characterize the overall sink of OH is to measure directly the ambient loss rate of OH, the total OH reactivity. To date, direct measurements of total OH reactivity have been either performed using a Laser-Induced Fluorescence (LIF) system ("pump-and-probe" or "flow reactor") or the

Comparative Reactivity Method (CRM) with a Proton-Transfer-Reaction Mass Spectrometer (PTR-MS). Both techniques require large, complex and expensive detection systems. This study presents a feasibility assessment for CRM total OH reactivity measurements using a new detector, a Gas Chromatographic Photoionization Detector (GC-PID). Such a system is smaller, more portable, less power consuming and less expensive than other total OH reactivity measurement techniques.

 Total OH reactivity is measured by the CRM using a competitive reaction between a reagent (here pyrrole) with OH alone and in the presence of atmospheric reactive molecules. The new CRM method for total OH reactivity has been tested with parallel measurements of the GC-PID and the previously validated PTR-MS as detector for the reagent pyrrole during laboratory experiments, plant chamber and boreal field studies. Excellent agreement of both detectors was found when the GC-PID was operated under optimum conditions. Time resolution (60-70 s), sensitivity (LOD 3-6 sg-1) and overall uncertainty (25% in optimum conditions) for total OH reactivity were similar to PTR-MS based total OH reactivity measurements. One drawback of the GC-PID system was the steady loss of sensitivity and accuracy during intensive measurements lasting several weeks, and a possible toluene interference. Generally, the GC-PID system has been shown to produce closely comparable results to the PTR-MS and thus in suitable environments (e.g. forests) it presents a viably economical alternative for groups interested in total OH reactivity observations.© 2012 Author(s).

KEYWORDS: accuracy assessment; atmospheric chemistry; feasibility study; gas chromatography; gas phase reaction; hydroxyl radical; oxidant; sensitivity analysis; toluene .

www.atmos-meas-tech.net/5/2981/2012/

doi:10.5194/amt-5-2981-2012

207. Dolgorouky,C., Gros,V., Sarda-Esteve,R., **Sinha,V.**, Williams,J., Marchand,N., Sauvage,S., Poulain,L., Sciare,J., and Bonsang B. **(2012)** : T*otal OH reactivity measurements in Paris during the 2010 MEGAPOLI winter campaign*, **Atmos. Chem. Phys.**, **12, 9593-9612,**

ABSTRACT: Hydroxyl radicals play a central role in the troposphere as they control the lifetime of many trace gases. Measurement of OH reactivity (OH loss rate) is important to better constrain the OH budget and also to evaluate the completeness of measured VOC budget. Total atmospheric OH reactivity was measured for the first time in an European Megacity: Paris and its surrounding areas with 12 million inhabitants, during the MEGAPOLI winter campaign 2010. The method deployed was the Comparative Reactivity Method (CRM). The measured dataset contains both measured and calculated OH reactivity from CO, NO_x and VOCs measured via PTR-MS, GC-FID and GC-MS instruments. The reactivities observed in Paris covered a range from 10 s^{-1} to 130 s^{-1}, indicating a large loading of chemical reactants. The present study showed that, when clean marine air masses influenced Paris, the purely local OH reactivity (20 s^{-1}) is well explained by the measured species. Nevertheless, when there is a continental import of air masses, high levels of OH reactivity were obtained (120–130 s^{-1}) and the missing OH reactivity measured in this case jumped to 75%. Using covariations of the missing OH reactivity to secondary inorganic species in fine aerosols, we suggest that the missing OH reactants were most likely highly oxidized compounds issued from photochemically processed air masses of anthropogenic origin.

KEYWORDS: volatile organic-compounds; gas-phase reactions; positive matrix factorization; new-york-city; ptr-ms; atmospheric chemistry; source apportionment; photochemical data; urban atmosphere; high-resolution

http://www.atmos-chem-phys.net/12/9593/2012/acp-12-9593-2012.html
doi:10.5194/acp-12-9593-2012

208.Rajkumar, V., Aslam, N.A., Reddy, C., Babu, S.A. (2012) *Unactivated norbornenes in [3+2] cycloadditions: Remarkably stereo-controlled entry into norbornane-fused spirooxindolopyrrolidines,spiro-1,3-indandionolylpyrrolidines,and spirooxindolopyrrolizidines* . **Synlett, (4), pp. 549-556.**

ABSTRACT: 1,3-dipolar cycloaddition reactions of azomethine ylides with unactivated norbornene dipolarophiles and a highly diastereoselective synthesis of the novel norbornane-fused spirooxindolo-pyrrolidines, spiroacenaphthylenolylpyrrolidines, spiro-1,3-indan-dionolylpyrrolidines, and

spirooxindolopyrrolizidines having an array of stereocenters are reported. The stereoselective synthesis of spirooxindolopyrrolizidines with eight stereocenters was demonstrated. Single-crystal X-ray structural analyses were performed to unambiguously establish the structure and stereochemistry of the key products. © Georg Thieme Verlag Stuttgart · New York.

KEYWORDS: pyrrolizidine derivative; spiro 1,3 indandionolylpyrrolidine derivative; spirooxindolopyrrolidine derivative; spirooxindolopyrrolizidine derivative; unclassified drug, article; crystal structure; cycloaddition; Diels Alder reaction; drug structure; drug synthesis; high temperature; stereochemistry; structure analysis

https://www.thieme-connect.com/ejournals/abstract/10.1055/s-0031-1290342

DOI: 10.1055/s-0031-1290342

209. Giovannetti, G., **Kumar, Sanjeev**., Pouget, J.-P., Capone, M.(**2012**) U*nraveling the polar state in TMTTF*$_2$*-PF*$_6$ *organic crystals .***Physical Review B - Condensed Matter and Materials Physics, 85 (20), art. no. 205146, .**

ABSTRACT: Combining density-functional theory and many-body approaches we investigate the origin of the ferroelectric phase generally observed in TMTTF$_2$-X organic crystals. We solve by means of mean-field theory and exact diagonalization a two-dimensional tight-biding model built from density-functional theory calculations and we show that short-range interactions stabilize a dimerized charge-ordered state in a wide range of parameters. Two different charge-ordering patterns are found; these correspond to those observed for X=PF$_6$ and X=SCN. In the former case, a lattice dimerization couples with the charge ordering, leading to a polarization. Due to the interplay between charge and magnetic ordering, such polarization appears to be magnetically driven, thus revealing TMTTF$_2$-PF$_6$ as a multiferroic material. © 2012 American Physical Society.

http://prb.aps.org/abstract/PRB/v85/i20/e205146

DOI:10.1103/PhysRevB.85.205146

210. Kumari, Amrita., **Dorai, K. (2012)** *Using the 19F NMR chemical shift anisotropy tensor to differentiate between the zigzag and chiral forms of fluorinated single-walled carbon nanotubes* . **Journal of Physical Chemistry A, 115 (24), pp. 6543-6550**.

ABSTRACT: The structural characterization of different kinds of zigzag and chiral single-walled carbon nanotubes (SWNTs) has been investigated theoretically using 19F NMR spectroscopy. The chemical shift anisotropy (CSA) tensor is computed at different levels of theory for the 19F nuclei in different forms of functionalized fluorinated carbon nanotubes (CNT). A set of fluorine CSA parameters comprising the span, skew, and isotropic chemical shift is computed for each form of the fluoronanotubes and multidimensional CSA parameter correlation maps are constructed. We show that these correlations are able to clearly distinguish between the chiral and zigzag forms of fluorinated carbon nanotubes (F-SWNTs). Implications for solid-state and liquid-state NMR experiments are discussed. © 2011 American Chemical Society.

KEYWORDS: Chemical shift anisotropy; Fluorinated carbon nanotubes; Functionalized; Isotropic chemical shifts; Liquid state; NMR chemical shifts; Parameter correlation; Structural characterization, Anisotropy; Chemical shift; Fluorine; Nuclear magnetic resonance spectroscopy; Tensors, Single-walled carbon nanotubes (SWCN), carbon nanotube; fluorine, anisotropy; article; chemistry; nuclear magnetic resonance spectroscopy; quantum theory; standard, Anisotropy; Fluorine; Magnetic Resonance Spectroscopy; Nanotubes, Carbon; Quantum Theory; Reference Standards

http://pubs.acs.org/doi/abs/10.1021/jp2033388

DOI:10.1021/jp2033388

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212. Neal S Gupta (2011) Chitin; formation and diagnosis series .**Topics in Geobiology, Vol. 34.**

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KEYWORDS: Arthropod;Biogeochemistry;Geochemistry;Macromolecule;-Paleontology

ISBN: 978-90-481-9683-8 (Print) 978-90-481-9684-5 (Online)

http://www.springer.com/earth+sciences+and+geography/book/978-90-481-9683-8

211. A.K. Jain., H. Chandrasekharan., **Visakhi. P.**, HansRaj and Nabi Hasan (Ed.,) (2011) Proceedings of National Conference of Agricultural Librarians and User Community 2011 *on" Agricultural Libraries in the Knowledge Web ",*held during 24-25th February 2011 by e-Granth, IARI and AALDI. Indian Agricultural Research Institute : New Delhi.

213. S.K. Paul (2011) *Design, Synthesis, and Self-assembly of Functionalized Soft Materials: Discotic Liquid Crystals*: **Science and Applications, publ. VDM Verlag Dr. M̈ller .**

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KEYWORDS : Science, Chemistry, Organic

http://www.campusbooks.com/books/science/chemistry/organic/9783639153347_Santanu-Pal-Iiser-Mohali_Design-Synthesis-and-Selfassembly-of-Functionalized-Soft.htm

(ISBN: 9783639153347)

214. Veeranjaneyulu., Rabindra K., Mahapatra., **P. Visakhi** (2012) (Ed.,) *Library Services in the Knowledge Web.(* Collection of papers in honour of Dr Stanley Madan Kumar) 2012, New India Publishing Agency, New Delhi.
www.theindianbookshop.com/-services-in-the-knowledge-web.
ISBN 13: 9789381450192

215. Satish Shirali., **Harkrishan Lal Vasudeva (2011)** *Multivariable Analysis*.**, Springer London Ltd**

Book Description : This book provides a rigorous treatment of multivariable differential and integral calculus. Implicit function theorem and the inverse function theorem based on total derivatives is explained along with the results and the connection to solving systems of equations. There is an extensive treatment of extrema, including constrained extrema and Lagrange multipliers, covering both first order necessary conditions and second order sufficient conditions. The material on Riemann integration in n dimensions, being delicate by its very nature, is discussed in detail. Differential forms and the general Stokes' Theorem are expounded in the last chapter. With a focus on clarity rather than brevity, this text gives clear motivation, definitions and examples with transparent proofs. Much of the material included is published for the first time in textbook form, for example Schwarz' Theorem in Chapter 2 and double sequences and sufficient conditions for constrained extrema in Chapter 4. A wide selection of problems, ranging from simple to more challenging, are included with carefully formed solutions. Ideal as a classroom text or a self study resource for students, this book will appeal to higher level undergraduates in Mathematics.

KEYWORDS : Advanced Calculus, Multivariable Calculus, Real Analysis

http://mathdl.maa.org/mathDL/19/?pa=reviews&sa=viewBook&bookId=71924

ISBN-10: 0857291912

216 I.B.S.Passi (Ed.,) (2012) *Symmetry: A multi-disciplinary perspective*, **Ramanujan Lecture Notes Series, Vol. 16. (142 pages): International Press of Boston, Inc, Boston**

ISBN-13: 978-1571462473

217. Meera Nanda (2011) *The God Market: How Globalization is Making India More Hindu* **(The North American edition, with a new extended introduction), Monthly Review Press. New York.** (Random House Publishers Indian PVT Ltd., for 2009 Original Edition)

Book Description: Conventional wisdom says that integration into the global marketplace tends to weaken the power of traditional faith in developing countries. But, as Meera Nanda argues in this path-breaking book, this is hardly the case in today's India. Against expectations of growing secularism, India has instead seen a remarkable intertwining of Hinduism and neoliberal ideology, spurred on by a growing capitalist class. It is this "State-Temple-Corporate Complex," she claims, that now wields decisive political and economic power, and provides ideological cover for the dismantling of the Nehru-era state-dominated economy. According to this new logic, India's rapid economic growth is attributable to a special "Hindu mind," and it is what separates the nation's Hindu population from Muslims and others deemed to be "anti-modern." As a result, Hindu institutions are replacing public ones, and the Hindu "revival" itself has become big business, a major source of capital accumulation. Nanda explores the roots of this development and its possible future, as well as the struggle for secularism and socialism in the world's second-most populous country.

http://books.google.co.in/books?id=A3M6zct0L50C&printsec=frontcover& source= gbs_ge_summary_r&cad=0#v=onepage&q&f=false

ISBN :978-1-58367-249-5

218. Pathania, M.S., Veeranjaneyulu, K., Prem Singh., **Visakhi .P** (Eds) **(2011)** . "*Transformation of Agricultural libraries in Collaborative Era*" . National Conference on Agricultural Librarians & User Community (NCALUC -2011).,held during 17th -19th Nov. 2011 at : Dr.Y.S.Parmar University of Horticulture & Forestry, NAUNI, SOLAN ., B.S. Publication, Hyderabad

ISBN: 978-93-81075-59-3

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