

## CHEMICAL, PHYSICAL AND MATHEMATICAL SCIENCES

### CMPSD No. 1 HYBRID 'SINTA' PAPAYA (*Carica papaya*) RIPENING FRUIT EXHIBITS UNIQUE ACC SYNTHASE 1 GENES

Marie-Sol P. Hidalgo<sup>1</sup>, Antonio C. Laurena<sup>1</sup>,  
J. Botella<sup>2</sup> and Evelyn Mae Tecson-Mendoza<sup>1</sup>

<sup>1</sup>Institute of Plant Breeding, College of Agriculture  
University of the Philippines Los Baños, College, 4031 Laguna

<sup>2</sup>Department of Botany, School of Life Sciences  
University of Queensland, Brisbane, Qld.

Five ripening-related ACC synthase cDNAs have been cloned from 80% ripe papaya cv. Sinta by reverse transcription-PCR using Ole primers. The DNA sequences show that the clones contain the ACC synthase active site and four amino acid residues invariant among ACC synthases and aminotransferases. Southern blot analysis indicates that all five clones came from only one gene existing as a single copy in the papaya genome. Sequence analysis indicates that all five isoforms arise from a single gene through alternative splicing mechanisms. Clone 2 is the longest transcript and contains all common exons and three alternative exons. Clones 3 and 4 contain common exons and one alternative exon each, while clone 1 contains only the common exons. All the alternative exons are present in the N-terminal of the gene. Clone 5 was shown to be due to cloning artifacts and not a unique cDNA fragment, thus, there are only four isoforms of ACC synthase mRNA. Sinta ACC synthase cDNAs were of the *capaccs* 1 type and are most closely related to AJ277160, a 1.4 kb *capaccs* 1-type DNA from Eksotika papaya. No *capaccs* 2-type genes were cloned from Sinta. This is the first report of alternative splicing in ACC synthase genes.

**Keywords:** Sinta, ACC synthase, DNA sequence

### CMPSD No. 2 COMPUTATIONAL ANALYSIS OF CATION- $\pi$ INTERACTIONS IN CRY PROTEINS OF *Bacillus thuringiensis*

Edwin P. Alcantara

National Institute of Molecular Biology and Biotechnology  
University of the Philippines Los Baños, College, 4031 Laguna

Cation- $\pi$  interaction is increasingly recognized as an important non-covalent interaction in structural biology. It is thought to be important in protein stability, molecular interaction, and other biological functions. An energy-based algorithm was adopted to

identify significant cation- $\pi$  pairs in Cry proteins from *Bacillus thuringiensis*. Four Cry proteins (CryIAa, Cry2A, Cry3A, and Cry3B) with known three-dimensional structures were analyzed for the presence of cation- $\pi$  interactions. Results show that energetically significant cation- $\pi$  pairs exist in the molecular structure of the Cry proteins. Cry2A and CryIAa had the highest and lowest number of cation- $\pi$  pairs, respectively. Majority of the energetically significant cation- $\pi$  pairs in CryIAa (83.3%) and Cry2A (84.6%) was of intradomain location but not in Cry3A (54.5%) and Cry3B (44.4%). Domain II of Cry2A contained the highest number of intradomain cation- $\pi$  interaction represented by arginine and phenylalanine, arginine and tyrosine, and arginine and tryptophan pairs. Among the Cry proteins examined, only CryIAa do not have cation- $\pi$  interactions in domain III and that lysine was not involved in cation- $\pi$  pairings anywhere in the structure of CryIAa. The strongest cation- $\pi$  pair was observed between lysine 209 and phenylalanine 206 in domain I of Cry3A with the electrostatic component of the binding energy,  $E_{\text{el}} = -7.79$  kcal/mol.

**Keywords:** cation- $\pi$  interaction, *Bacillus thuringiensis*, Cry proteins

**CMPSD No. 3 CLONING AND CHARACTERIZATION OF THE GENE ENCODING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE IN COCONUT (*Cocos nucifera* L.)**

**Hazel R. Lapis-Gaza, Merlyn S. Mendioro, Rita P. Laude, Ma. Jamela R. Revilleza, Ivan Marcelo A. Duka, M.G.Q. Diaz, Evelyn Mae Tecson-Mendoza and Antonio C. Laurena**

Genetics and Molecular Biology Laboratory, Institute of Biological Science  
University of the Philippines Los Baños, College, 4031 Laguna

RT-PCR strategy was employed to clone the gene encoding glyceraldehyde-3-phosphate dehydrogenase (gap) in coconut using a gene specific 20-mer primer pair. The sense primer has a 45.3°C melting temperature ( $T_m$ ) and 50% GC content. The antisense primer, on the other hand, has 48.3°C  $T_m$ , 50% GC and a repeat in it. Using a modified Invitrogen's one-step TOPO-TA Cloning Kit, the 845 bp PCR product was inserted into a TOPO vector and was used in the transformation of *E. coli* DH5 $\alpha$ . Two positive clones were sequenced (H3 and H23). The partial cDNA sequence of H3 clone (designated as cocogapC1) contained 669 nucleotides with an ORF encoding 222 amino acids, corresponding a 24.4Kda polypeptide. Sequence alignment revealed that it has 72.9% nucleotide sequence homology and a 95.6% amino acid homology with those from other plant species' gap genes. On the other hand, the partial cDNA sequence of H23 clone (designated as cocogapC2) is composed of only 649 nucleotides with an ORF that encoded a polypeptide of 216 amino acid with 24.2KDa molecular weight. Alignment with other plant gap sequences showed that it has a 72.6% nucleotide sequence homology and 95.9%

amino acid homology. Regions associated with the metabolite function of NAD-gap were noted on both cocogapC1 and C2 deduced amino acid sequences. These regions include the putative NAD-binding domain from Thr-3 to Ala-114 and the putative catalytic-binding domain from Val-115 to Val-173. Alignment of the nucleotide and amino acid sequences of cocogapC1 and C2 revealed percent identities < 95%, (89.1% and 72.5%, respectively) thus, strongly suggesting that cocogapC1 and C2 are isoforms of the gene encoding glyceraldehyde-3-phosphate dehydrogenase.

**Keywords:** cloning, glyceradehyde-3-phosphate dehydrogenase, RT-PCR, isozymes, coconut

#### **CMPSD No. 4 THE PURIFICATION OF AN ENANTIOSELECTIVE MOLD LIPASE AND THE CLONING OF ITS GENE**

**Dominggus Malle<sup>1</sup>, Ma. Jamela R. Revilleza<sup>1</sup>, Antonio C. Laurena<sup>2</sup>,  
Milagros M. Peralta<sup>1</sup>, Gina O. Garingan<sup>1</sup> and Ivan Marcelo A. Duka<sup>3</sup>**

<sup>1</sup>Institute of Chemistry, College of Arts and Sciences (CAS)

<sup>2</sup>Institute of Plant Breeding, College of Agriculture

<sup>3</sup>Institute of Biological Sciences, CAS

University of the Philippines Los Baños, College, 4031 Laguna

An *Aspergillus niger* exolipase was purified via sequential ultrafiltration and ion-exchange chromatography. The SDS-PAGE profile revealed the presence of two bands while the native gel, a single band. The two-step protocol has resulted in a 27-fold increase in purity. The purified extract was found to be predominantly S(+)-enantioselective in the hydrolysis of the racemic mixture of a model compound of an aryl butyl ester after HPLC analysis of the hydrolysates using a chiral column. The enzyme was characterized to have optimum activity at neutral pH and at 30-35°C.

Alignments of related fungal lipases revealed the presence of a conserved region, which facilitated the identification of a gene specific primer, together with oligo dT as the other primer, for reverse transcription-polymerase chain reaction (RT-PCR). The reaction produced a fragment, which after cloning and sequencing revealed a putative lipase encoding segment.

The transformant bearing the RT-PCR product was grown in liquid culture and evaluated to express lipase, a fusion protein, with an activity of 0.83 U/mL, detected after 24 h, not found in *A. niger* culture.

**Keywords:** lipase, enantioselective, *Aspergillus niger*

**CMPSD No. 5 PURIFICATION AND PARTIAL CHARACTERIZATION  
OF A LECTIN FROM THE LEAVES OF *Pithecellobium dulce* (Roxb.) Benth**

**Ana Christina L. Opina, Marivic S. Lacsamana and Florina E. Merca**

Institute of Chemistry, College of Arts and Sciences  
University of the Philippines Los Baños, College, 4031 Laguna

Lectins are sugar-binding proteins or glycoproteins of non-immune origin that can precipitate glycoconjugates and agglutinate cells. They have been proven to be powerful tools in biological, biochemical and medical research. This study reports the purification and partial characterization of a lectin in the leaves of *Pithecellobium dulce* (Roxb.) Benth.

The leaf lectin was extracted using 0.02 M phosphate buffered saline (pH 7.2) and purified using sequential ammonium sulfate fractionation and gel filtration on Sephadex G-200. The native lectin exhibited a molecular mass of about 79 kD on gel filtration using Sephadex G-200. SDS-PAGE revealed two protein bands with molecular masses estimated to be 66 and 45 kD, respectively. It showed hemagglutinating activity toward human erythrocytes from all blood types and animal erythrocytes such as calf, carabao, goat, rabbit and swine. The native lectin was found to be a glycoprotein containing 18.9% total sugars.

The results presented indicate the potential of the leaves of *Pithecellobium dulce* (Roxb.) Benth. as a readily available and cheap source of lectins.

**Keywords:** lectin, glycoprotein

**CMPSD No. 6 ANTITUBERCULAR COUMARIN FROM THE  
FRUIT JUICE OF *Morinda Citrifolia***

**Jonel P. Saludes<sup>1</sup>, M.J. Garson<sup>2</sup> and S.G. Franzblau<sup>3</sup>**

<sup>1</sup>Department of Chemistry, University of San Agustin, Iloilo City

<sup>2</sup>Department of Chemistry, The University of Queensland, Brisbane, QLD, Australia

<sup>3</sup>Institute for Tuberculosis Research, University of Illinois at Chicago, Illinois, USA

Ethnobotanical study of Degener reported that Hawaiians use a concoction called *auniki awa*, prepared using the fruit of *Morinda citrifolia* (noni) as a component, to treat tuberculosis. Noni is unique because it is associated with many healing properties that characterize claims for its efficacy while only a few investigations have been conducted to scientifically validate these claims. To date, only one group has investigated the antitubercular potential of this plant.

This present study subjected the fruit juice of a Philippine collection of this plant to *in vitro* assay against *Mycobacterium tuberculosis* H37Rv, the causative organism of tuberculosis. Results showed that it possesses 82% inhibitory activity against the test organism at 100 µg/mL concentration while its CHCl<sub>3</sub> fraction exhibited 100% inhibition at the same concentration. Purification of this CHCl<sub>3</sub> fraction through stepwise normal phase gravity column chromatography using CHCl<sub>3</sub> and EtOAc as mobile phase yielded white needle-like crystals. Through a combination of melting point and spectral analysis (ultraviolet: <sup>1</sup>H, <sup>13</sup>C, gradient enhanced heteronuclear single quantum coherence and heteronuclear multiple bond correlation nuclear magnetic resonance spectroscopy; and mass spectrometry) and comparison with published data, it was identified as a coumarin. We report its first isolation in *M. citrifolia* and present the spectral data, structure and antitubercular activity of this compound.

**Keywords:** tuberculosis, *Morinda citrifolia*, noni, *in vitro*, *Mycobacterium tuberculosis* H37Rv, melting point, spectral analysis, coumarin

**CMPSD No. 7      PHYSICO-CHEMICAL PROPERTIES OF  
N,O-CARBOXYMETHYL CHITOSAN AND ITS USE AS A COATING  
TO EXTEND THE SHELF-LIFE OF MANGOES (*Mangifera indica* L.)**

**Gladdys D. Dizon<sup>1</sup>, Veronica C. Sabularse<sup>1</sup>, Milagros M. Peralta<sup>1</sup>  
and Edralina P. Serrano<sup>2</sup>**

<sup>1</sup>Institute of Chemistry

<sup>2</sup>Postharvest Horticulture Training and Research Center  
University of the Philippines Los Baños, College, 4031 Laguna

N,O-carboxymethyl chitosan (NOCC) was prepared by mercerization and etherification. The product was film forming and had the following characteristics: percent solubles – 53.6%, degree of substitution (DS) – 0.45, molecular weight –  $6.76 \times 10^4$  and degree of polymerization (DP) – 355,789. The prepared NOCC was used as a coating for shelf-life extension of mangoes. Physicochemical changes in the coated mangoes were monitored during storage while titratable acidity, total soluble solids and pH were measured on the first and last day of storage. The NOCC-coated mangoes showed an increase in titratable acidity and a decrease in total soluble solids, pH as well as least weight loss, shriveling and softening. The coating containing one percent carboxymethyl chitosan plus additives retained skin greenness of mangoes. Incidence of disease and infection was low in the coated fruits indicating the potential of NOCC as an antimicrobial agent against anthracnose disease. These results indicated that NOCC may be used as coating for storage life extension of mangoes.

**Keywords:** N,O-carboxymethyl chitosan, chitosan, coating

**CMPSD No. 8      COMPARISON OF TWO ELISA-BASED SCREENING  
AND MINICOLUMN TEST KITS WITH LIQUID CHROMATOGRAPHY  
FOR THE DETERMINATION OF AFLATOXINS IN CORN:  
A PRELIMINARY REPORT**

Rosario H. Arim<sup>1</sup>, L.A. Esteves<sup>2</sup>, C.A. Ferolin<sup>1</sup>, V.M. Bunyi<sup>2</sup> and R. P. Ramirez<sup>1</sup>

<sup>1</sup>Food and Nutrition Research Institute  
Department of Science and Technology, Bicutan, Taguig, 1631 Metro Manila  
<sup>2</sup>Bureau of Postharvest Research and Extension  
Department of Agriculture, Muñoz, Nueva Ecija

Two enzyme-linked immunosorbent assay (ELISA)-based screening and a developed minicolumn test kits performance were compared with a quantitative method for aflatoxin determination in corn. The samples analyzed included one set of artificially-contaminated corn containing different aflatoxin levels (0, 10, 20 and 50 µg aflatoxin B<sub>1</sub>/kg sample), and a set of naturally-contaminated corn samples containing similar aflatoxin levels. Data of the analysis with each test kit were evaluated and compared with the liquid chromatography data of the test samples. Results showed that both the two ELISA-based test kits gave positive responses of 71% and the "lahar" minicolumn test kit, 83.3%. The performance of the locally-developed aflatoxin test kit which utilizes a "lahar" minicolumn is comparable to that of the commercial test kits.

**Keywords:** ELISA, minicolumn, aflatoxins, liquid chromatography

**CMPSD No. 9      ANALYSIS OF AMYLOSE CONTENT OF NINE (9)  
TRADITIONAL BASMATI RICE VARIETIES CULTIVATED  
UNDER PHILIPPINE CONDITIONS**

Hazel B. Alfon<sup>1</sup>, A.H. Bhatti<sup>1</sup>, Henry M. Corpuz<sup>2</sup>, Q.D. dela Cruz<sup>2</sup>  
and Leocadio S. Sebastian<sup>2</sup>

<sup>1</sup>Institute of Graduate Studies, Central Luzon State University  
Science City of Muñoz, Nueva Ecija  
<sup>2</sup>Philippine Rice Research Institute Central Experiment Station  
Science City of Muñoz, Nueva Ecija

Basmati rice cultivars have their origin in India and Pakistan. They are characterized by long slender grain, strong aroma, and intermediate amylose content.

Amylose content (AC) is one of the grain quality characters that vary from country

to country. This study was undertaken to determine the effect of Philippine conditions on the amylose content of nine (9) introduced Basmati rice cultivars that were planted in the experimental field at Central Luzon State University, Nueva Ecija during the wet season of 2001.

Percent AC (%AC) was determined using an Autoanalyzer following the method developed by Juliano (1971) with modifications. Results indicated that eight (8) out of nine (9) cultivars had low AC while only one (1) had intermediate amylose content.

**Keywords:** Basmati cultivar, amylose content, Philippine conditions

### **CMPSD No. 10 REVIEW OF VALUABLES FOR AMYLOSE CONTENT ANALYSIS OF MILLED RICE**

**Henry M. Corpuz<sup>1</sup>, Hazel B. Alfon<sup>1</sup>, A.H. Bhatti<sup>2</sup>, Edilberto D. Redoña<sup>1</sup>  
and Leocadio S. Sebastian<sup>1</sup>**

<sup>1</sup>Philippine Rice Research Institute, Science City of Muñoz, Nueva Ecija

<sup>2</sup>Central Luzon State University, Science City of Muñoz, Nueva Ecija

Amylose and amylopectin are anhydroglucose units that are the major components of rice grains. Amylose content is one of the determinants for cooking and eating qualities of rice, thus, its value is a crucial indicator of rice grain quality.

Iodine staining method developed by Juliano (1971) is the widely accepted procedure for routine quantification of amylose in milled rice. It is also the protocol approved by the Rice Technical Working Group of the National Seed Industry Council, Department of Agriculture. Using this method, a preliminary test on different brand combinations and different defatting procedures was undertaken in the Analytical Services Laboratory of PhilRice. The test showed that alteration of results may come from factors such as the brand of amylose and amylopectin standards, brand combinations for amylose and amylopectin mixtures, and the defatting procedure for standard checks (IR8, IR24, IR29, IR64).

**Keywords:** amylose, amylopectin, iodine staining method

**CMPSD No. 11 SURFACE STUDIES AND BIOMIMETIC PROPERTIES  
OF A PIEZOELECTRIC CAFFEINE SENSOR BASED ON  
MOLECULARLY IMPRINTED POLYMER**

**Benilda S. Ebarvia<sup>1</sup>, Christina A. Binag<sup>2</sup> and Fortunato B. Sevilla III<sup>2</sup>**

<sup>1</sup>Industrial Technology and Development Institute, Department of Science and  
Technology, Bicutan, Taguig, 1631 Metro Manila

<sup>2</sup>Thomas Aquinas Research Center, University of Santo Tomas, España, Manila

The measurement of caffeine is important in water quality monitoring, since it could be used as a marker for human fecal contamination in surface waters. In this study, the feasibility of a piezoelectric quartz caffeine sensor based on molecularly imprinted polymer (MIP) was explored.

The MIP was prepared by co-polymerization of methacrylic acid and ethyleneglycol dimethacrylate with caffeine as the template molecule, chloroform as the solvent and azobisisobutyronitrile as the initiator followed by Soxhlet extraction of caffeine using methanol-acetic acid. The caffeine sensor was devised by spin-coating onto one side of the 10 MHz AT-cut quartz crystal the MIP suspension in cyanoacrylate ester-tetrahydrofuran (6:2:1 w/w/v) solution. The coated crystal set in a fabricated cell with its electrode connected to a Pierce oscillator circuitry and a frequency counter was used for measurement of resonant frequency of the quartz when it was in contact with the solution. The sensor exhibited a linear relationship between frequency shift and caffeine concentration in the range of  $1 \times 10^{-6}$  up to 1 mg/mL. It has a sensitivity of about 61 Hz/ln (conc. mgmL<sup>-1</sup>).

Surface studies using SEM and XPS were conducted in order to elucidate the imprinting of the caffeine molecule. The SEM micrograph and XPS spectra confirmed the removal of caffeine by Soxhlet extraction in the imprinting process and the rebinding of caffeine to the MIP during the sensing process.

**Keywords:** caffeine, piezoelectric sensor, molecularly imprinted polymer

**CMPSD No. 12 ON THE INTRAMOLECULAR DISSOCIATION PATHWAYS  
OF FCOOCH<sub>2</sub>CH<sub>2</sub> IN THE GAS PHASE: A DFT STUDY 1. ENOL PATH**

**Wilfredo C. Chung<sup>1</sup> and E.W. Ignacio<sup>1</sup>**

<sup>1</sup>Department of Chemistry, College of Arts and Sciences, Northern Mindanao  
State Institute of Science and Technology, Ampayon, Butuan City

<sup>2</sup>Department of Chemistry, MSU-Iligan Institute of Technology, Tibanga, Iligan City

A ground-state intramolecular gas-phase dissociation pathway of ethyl



fluoroformyl radical cation ( $\text{FCOOCH}_2\text{CH}_2^+$ ) is uncovered using conventional *ab initio* and density functional molecular orbital theory calculations. Geometries are optimized using the 6-31G\* basis set. Electron correlation is incorporated by optimizing the geometries at the MP2 and B3LYP levels using the 6-31G\*\* basis set. Stationary points are characterized by frequency calculation at the same level of theory and basis set except for MP2 where only HF/6-31G\* corrections were applied. In a so-called enol path, the  $\alpha$ -distonic radical cation undergoes a barrierless isomerization to a more stable  $\gamma$ -distonic enol form  $\text{FC}^+(\text{OH})\text{OCH}_2\text{CH}_2$ . This is followed by a rate-determining self-induced cleavage of the ester linkage yielding  $\text{FCOOH} + \text{C}_2\text{H}_4^+$  in the second step of an Ei scheme which is at the same time the first step of an E1  $\beta$ -elimination mechanism. The enol pathway is terminated by a slow elimination of a proton from  $\text{C}_2\text{H}_4^+$  by  $\text{FCOOH}$  which acts as a base. The above conclusions are drawn from the results of density functional (UB3LYP/6-31g\*\*) calculations as the conventional *ab initio* treatment [UHF/6-31G\* and UMP2(Full)/6-31G\*\*//UHF/6-31G\*] gave erroneous energetics due to heavy spin-contamination of the wave function.

**Keywords:** enthyl fluoroformate, distonic radical cation, density functional theory, spin contamination, fluoroformic acid, *ab initio*, molecular orbital theory, reaction mechanism, Ei, E1

**Acronyms:** DFT - Density Functional Theory; MP2(Full) - Moller-Plesset correlation energy correction truncated at the 2nd order with all electrons included; B3LYP - Beckes Three Parameter Hybrid Method using the correlation functional of Lee, Yang and Parr; HF - Hartree-Fock (theory)

### **CMPSD No. 13      BROMIDE-SELECTIVE ELECTRODE BASED ON CONDUCTING POLYANILINE (PAn)**

**Karen S. Santiago<sup>1</sup> and Christina A. Binag<sup>2</sup>**

<sup>1</sup>Department of Chemistry, College of Science

<sup>2</sup>Graduate School

University of Santo Tomas, Manila 1008

Monitoring of inorganic anions in water samples is essential in order to determine if their level is within the allowable limit for human consumption. Hence, this study is aimed towards the development of a low cost  $\text{Br}^-$ -selective electrode using conducting PAn.

Galvanostatic polymerization (0.45 mA) of aniline (An). onto a Pt wire (0.25

cm<sup>2</sup>) for 15 minutes in a solution containing 2:1 mole ratio of An monomer and NaBr, was carried out to devise the sensor. It presented the following figures of merit: a sub-Nernstian response time of - 48.6 mV/pBr; a good linearity of 0.998 (r<sup>2</sup>) from 10<sup>-4</sup>-10<sup>-2</sup> M Br at an average response time of ~2 minutes at 3 replicates (RSD=3.61%).

The electrochemical, surface and elemental properties of PAN were likewise characterized via cyclic voltammetry (CV), Scanning Electron Microscopy (SEM) and X-ray Photoelectron Spectroscopy (XPS), respectively.

The Br<sup>-</sup>-selective electrode showed a promising response; however, various parameters are still under investigation for better performance enhancement.

**Keywords:** polyaniline, conducting polymer, Br, CV, SEM, XPS

#### **CMPSD No. 14      COMPUTER ELUCIDATION OF CHEMICAL REACTION MECHANISMS USING STOCHASTIC AND MOLECULAR ORBITAL METHODS**

**Ernesto J. del Rosario**

Institute of Chemistry, College of Arts and Sciences  
University of the Philippines Los Baños, College, 4031 Laguna

Computer elucidation of chemical reaction mechanisms may be done using stochastic and molecular orbital (MO) methods. The stochastic (Monte Carlo) method is usually applied to gas phase reactions consisting of several elementary steps. The molecular collision corresponding to each elementary step is simulated by picks of two sets of random numbers in the computer; one set selects the time interval between collisions and the other set picks the elementary step. The mechanism of the overall reaction is obtained in terms of the number of passes through each step, which in turn depends on the rate constant. The MO method involves computation of heats of formation ( $\Delta H_f$ ) and frontier molecular orbitals (FMO's) of reactants, possible intermediaries and products of the reaction; however, mechanistic evaluation is at best semi-quantitative.

The hydrogen-iodine reaction ( $H_2 + I_2 \longrightarrow 2HI$ ) was computer-simulated using the stochastic algorithm of Gillespie (1976). Plots of the number of molecules of H<sub>2</sub>, I<sub>2</sub>, HI, I and H vs. time (with specified initial numbers of reactant molecules) were prepared from the computer simulations at the following temperatures (in K) : 737.9, 721.0, 710.3, 666.7, 633.2, 520.1, 480.7 and 417.9. The equilibrium constant ( $K_{eq}$ ) was calculated at each temperature; all except one of the calculated  $K_{eq}$  values agreed with the literature values within 0.5%. The calculated heat of the reaction, which was obtained from the van't Hoff plot, was -12.1 kJ; the literature value is -9.5kJ.

The number of passes in the elementary steps composing the bimolecular, atomic and termolecular mechanisms were determined; the dissociation step for  $I_2$  was predominant at all temperatures. Among the three probable mechanisms for the formation of HI (excluding the dissociation of  $I_2$ ), the greatest contribution to the overall reaction came from the bimolecular step and was followed by the atomic and then the termolecular mechanisms.

The PM3 semi-empirical method was used to calculate the total and binding energies,  $\Delta H_f$  values, dipole moments and FMO's of the intermediates and oligomeric products of the glucose-glycine Maillard reaction. FMO calculations on the probable intermediates showed differences in the  $\Delta H_f$  values among the neutral form of the Schiff base, its enol forms, and the Amadori compound. The equilibrium constants were calculated for the following steps:



namely  $K_1 = 29$ ,  $K_2 = 4.2 \times 10^3$  and  $K_3 = 45.3 \times 10^{-8}$ .

The HOMO-LUMO energy gaps for the reactions among glucose, glycine and the Amadori compound were compared and showed that dimerization of the Amadori compound is the favored reaction. The cyclic and the non-cyclic forms of the dimeric product of the Amadori compound were also evaluated; further polymerization by the non-cyclic form rather than the cyclic form was preferred. Other six carbon products from the glucose-glycine Maillard reaction was examined. Based on the calculated  $\Delta H_f$  values of polymerization was favored while ring formation was disfavored.

**Keywords:** computer elucidation, chemical reaction mechanisms, molecular orbital methods, stochastic method, glucose, glycine, Amadori compound

### **CMPSD No. 15 ALL-SOLID-STATE POTENTIOMETRIC SENSOR FOR IODIDE BASED ON A MIXED $AgI/Ag_2S$ - EPOXY MEMBRANE**

**Joyce T. Tan and Fortunato B. Sevilla III**

Research Center for the Natural Sciences  
University of Santo Tomas, 1008 Manila

An all-solid-state approach to potentiometric sensor introduces technologically appealing features. The absence of the internal solution simplifies the design and allows this type of sensor to be used at any position. An all-solid-state potentiometric sensor for iodide was developed through the dispersion of mixed silver salts into an epoxy to produce a rigid and robust membrane. The sensing membrane consists of co-precipitated  $AgI$  and  $Ag_2S$  salts mixed with an Araldite epoxy mixture in a 6:1 w/w silver salt:epoxy

ratio. The sensor showed very good response characteristics to iodide ions as exhibited by its Nernstian response ( $m = -60.587 \text{ mV}/\log [I^-]$ ) and perfect correlation ( $r = 1.000$ ). The sensor's dynamic range spans 4.5 orders of magnitude with a low practical limit of detection at  $-6.5 \log a_{I^-}$ . The sensor's response is highly repeatable, reproducible and highly selective for iodide ions even in the presence of  $10^3 \text{ M } [Cl^-]$  as shown by its very low selectivity coefficient ( $K_{ij} = 2 \times 10^{-4}$ ). Application of this iodide sensor includes the following: 1) the determination and monitoring of iodide in foods (e.g. iodized salts) and 2) as a cyanide sensor since preliminary studies showed that the sensor is also selective to cyanide ions.

**Keywords:** all-solid-state potentiometric sensor, rigid membrane, iodide sensor

## CMPSD No. 16 DIMENSION OF POWERS OF SOME GRAPHS

Rowena T. Isla

Department of Mathematics, College of Science and Mathematics  
MSU-Iligan Institute of Technology, 9200 Iligan City

A unit graph in the Euclidean  $n$ -space  $R^n$  is a graph whose vertices are points in  $R^n$  and every pair of adjacent vertices  $x, y$  satisfy  $|x - y| = 1$  where  $|x - y|$  denotes the Euclidean distance between  $x$  and  $y$ . The smallest nonnegative integer  $n$  for which a graph  $G$  is a unit graph in  $R^n$  is called the *dimension* of  $G$ , denoted by  $\dim(G)$ .

Let  $G$  be a graph,  $k$  a positive integer. The  $k$ th power of  $G$ , denoted  $G^k$ , is the graph having the same vertex-set as  $G$  with vertices  $x, y$  adjacent in  $G^k$  whenever  $1 \leq d_G(x, y) \leq k$ , where  $d_G(x, y)$  denotes the distance between  $x$  and  $y$  in  $G$ .

This research study seeks to determine the dimension of the powers of some graphs. Among the major results obtained are the following:

1. If  $d(G)$  denotes the diameter of a connected graph  $G$  of order  $n > 1$ , then

$$\dim(G^{d(G)}) = n - 1.$$

2. If  $G$  is a connected graph of order  $n > 1$ , and  $1 \leq k < d(G)$ , then

$$\dim(G) \leq \dim(G^k) \leq \dim(G^{k+1}) \leq n - 1.$$

3. Let  $1 \leq k \leq n - 1$  and let  $P_n$  be the path of order  $n > 1$ . Then

$$\dim(P_n^k) = k \text{ if } k = 1, 2, n - 2, \text{ or } n - 1. \text{ If } n \geq 6 \text{ and } 3 \leq k \leq n - 3,$$

$$\text{then } k \leq \dim(P_n^k) \leq k + 1.$$

4. Let  $C_n$  be the cycle of order  $n$ . Then  $\dim(C_n^{\lfloor n/2 \rfloor}) = n - 1$ ,  
 $\dim(C_n^{2k-1}) = k$  and  $k \leq \dim(C_n^k) \leq n - \lfloor n/2 \rfloor$  when  
 $2 \leq k < \lfloor n/2 \rfloor$ .

5. If  $G$  is either the fan  $F_n$  or the wheel  $W_n$  of order  $n + 1$ , then  $\dim(G^2) = n$ .

**Keywords:** unit graph, dimension, power of a graph

### CMPSD No. 17 ON THE NUMBER OF INDUCED CYCLES IN THE COMPLEMENT OF GRAPHS

Joselito A. Uy

Mathematics Department  
MSU – Iligan Institute of Technology, 9200 Iligan City

Let  $G = (V(G), E(G))$  be a graph. The number of induced cycles in  $G$ , denoted by  $ic(G)$ , is the number of cycle-inducing subsets of  $V(G)$ . The complement of  $G$ , denoted by  $\bar{G}$ , has  $V(G)$  as its vertex set, but two vertices are adjacent in  $\bar{G}$  if and only if they are not adjacent in  $G$ . This paper studies the number of induced cycles in the complement of graphs. It particularly considers the complement of cycle  $C_n$ , generalized wheel  $W_{m,n}$ , path  $P_n$ , generalized fan  $F_{m,n}$ , and trees.

An explicit formula for  $ic(\bar{C}_n)$  in terms of  $n$  is established. This formula is useful in determining  $ic(\bar{G})$ , where  $G$  is a graph which has an induced cycle as a subgraph. Its usefulness is demonstrated in counting the number of induced cycles in the complement of generalized wheels.

An exact expression for  $ic(\bar{P}_n)$  in terms of  $n$  is found. This expression aids in deriving  $ic(\bar{G})$ , where  $G$  is a graph which has an induced path as a subgraph. Its importance is shown in finding the number of induced cycles in the complement of generalized fans.

Let  $T$  be a tree. This paper characterizes the existence of 4-cycles in  $\bar{T}$ . It shows that  $\bar{T}$  has no induced cycle of length greater than 4. Finally, it gives some lower and upper bounds for  $ic(\bar{T})$  in terms of order, stability number and maximum degree of  $T$ .

**Keywords:** graph, complement, cycle, induced cycle, generalized wheel, path, generalized fan, and tree

**CMPSD No. 18 DETERMINING COMMUTATIVITY AND NILPOTENCY OF A FINITE GROUP FROM ITS ORDER**

**Jose Maria P. Balmaceda**

Department of Mathematics, College of Science  
University of the Philippines Diliman, 1101 Quezon City

If a finite group contains a prime number of elements, then the group is cyclic, and hence unique up to isomorphism. Are there other integers for which the only groups of these orders are cyclic? The answer is yes; and a characterization is given by the following: Every group of the order  $N$  is cyclic if and only if  $N = p_1 p_2 \dots p_r$ , where  $p_i$  are distinct primes and  $p_i$  does not divide  $p_j - 1$  for all  $i, j$ . Surprisingly this result can be extended to obtain analogous theorems characterizing those integers  $N$  for which every group of order  $N$  is abelian or nilpotent. In this paper we present elementary proofs of these analogues, using the structure of the maximal subgroups of the group and their embedding in the whole group to obtain a contradiction by counting arguments.

**Keywords:** finite group, group order, classification, cyclic group, abelian group, nilpotent group, Euler phi-function, maximal subgroups

**CMPSD No. 19 THE SH<sub>1</sub> INTEGRAL IN A LOCALLY CONVEX TOPOLOGICAL VECTOR SPACE**

**Rolando N. Paluga**

Department of Mathematics, MSU, Marawi City

Recently, the author defined the Henstock integral of a function which takes its values in a topological vector space. Henstock integrability of a function  $f: [a, b] \rightarrow X$ , where  $X$  is a complete topological vector space, had been shown to be equivalent to the existence of a function  $F: [a, b] \rightarrow X$  satisfying the condition that for every neighborhood  $U$  of the zero vector  $\theta$ , there exists a positive function  $\delta$  on  $[a, b]$  such that if  $P = \{([x_{i-1}, x_i], x_i) : 1 \leq i \leq n\}$  is a  $\delta$ -fine tagged partition of  $[a, b]$ , there exist open sets  $U_1, U_2, \dots, U_n$  with  $\sum_{i=1}^n U_i \subseteq U$  such that  $F(x_i) - F(x_{i-1}) - (x_i - x_{i-1})f(t_i) \in U_i$  for all  $i$ . If we impose further that the open sets  $U_i$  are neighborhoods of the zero vector  $\theta$ , then the corresponding integral is called the strongly Henstock integral.

In this study, we considered a locally convex topological vector space and defined the SH<sub>1</sub> integral. This integral is obtained by imposing the additional condition the open sets  $U_i$  mentioned above are multiples of the open set  $U$ . It is shown that the SH<sub>1</sub> integral of a function, if it exists, is unique. Other results obtained included linearity of the integral, and the integrability on the subintervals. Further, it is shown that for Banach-valued

functions, the  $SH_1$  integral is equivalent to the HL integral defined by Cao.

**Keywords:** topological, vector, locally, convex, Henstock,  $SH_1$ -integral, Banach

## CMPSD No. 20      ON GRAPHS WHICH INDUCE THE EXCLUDED POINT TOPOLOGY

Sergio R. Canoy Jr.

Department of Mathematics, College of Science and Mathematics  
MSU-Iligan Institute of Technology, 9200 Iligan City

Let  $\tau$  be a topology on a finite nonempty set  $X$ . A natural way of constructing a graph  $G$  with vertex set  $V(G) = X$  is given as follows: For each pair of distinct elements  $x$  and  $y$  of  $X$ ,  $[x,y] \in E(G)$  (the edge set of  $G$ ) if and only if  $U \cap V = \emptyset$  for all open sets  $U$  and  $V$  with  $x \in U$  and  $y \in V$ . In other words, two distinct elements  $x$  and  $y$  of  $X$  are non-adjacent if and only if there exist disjoint open sets  $U$  and  $V$  such that  $x \in U$  and  $y \in V$ . This kind of construction was introduced by Diesto and Gervacio.

Interestingly, a topological space can be constructed from given a graph  $G = (V(G), E(G))$ . Indeed, a topology can be generated because the family consisting of sets  $F(A) = V(G) \setminus N(A)$ , where  $N(A) = A \cup \{x \in V(G) : [x,a] \in E(G) \text{ for some } a \in A\}$ , and  $A$  is subset of  $V(G)$ , forms a base for some topology on  $V(G)$ . This unique topology, denoted by  $\tau(G)$ , is referred to as the topology induced by the graph  $G$ .

In this study, we showed that for some restrictions on the order, the star and the wheel graphs both induce the excluded point topology. Furthermore, the study had come up with following main results:

(1) If  $G$  is a graph of order  $n \geq 4$ , then  $\tau(G)$  is an excluded set topology on  $V(G)$  if and only if the following conditions hold:

(a) there exists a nonempty proper subset  $A$  of  $V(G)$  such that  $[p,x] \in E(G)$  for every  $x \in V(G) \setminus \{p\}$  implies that  $p \in A$ ; and

(b) for each pair of vertices  $x, y \in V(G) \setminus \{p\}$  with  $[x,y] \in E(G)$ , there exist  $z \in A_y$  and  $w \in A_x$  such that  $[x,z], [y,w] \in E(G)$ , where  $A_y = \{s : s, y \text{ and } [s,y] \notin E(G)\}$ .

(2) The induced topology  $\tau(G)$  is an excluded point topology on  $V(G)$  if and only if the following conditions are satisfied:

(a) there exists exactly one vertex  $p \in V(G)$  such that  $[p,x] \in E(G)$  for every  $x \in V(G) \setminus \{p\}$ ; and

- (b) for each pair of vertices  $x, y \in V(G) \setminus \{p\}$  with  $[x, y] \in E(G)$ , there exist  $z \in A_x$  and  $w \in A_y$  such that  $[x, z], [y, w] \in E(G)$ .

**Keywords:** graph, vertex, star, wheel, topology, base, excluded

## CMPSD No. 21 ON THE MCSHANE INTEGRAL IN TOPOLOGICAL VECTOR SPACE

Rolando N. Paluga<sup>1</sup> and Sergio R. Canoy Jr.<sup>2</sup>

<sup>1</sup>Department of Mathematics  
Mindanao State University, Marawi City

<sup>2</sup>Department of Mathematics  
College of Science and Mathematics  
MSU-Iligan Institute of Technology, 9200 Iligan City

The Lebesgue integral has been considered by a lot of mathematicians as the official or standard integral in mathematical research. This integral overcomes some of the defects of the Riemann integral. However, the problem with Lebesgue's integral is that it is not easy to understand. One has to master a considerable amount of measure theory before he can fully understand it. Also, such an integral does not inherit the naturalness of the Riemann integral.

In the late 1960's, E.J. McShane defined a Riemann-type integral and proved that this integral is equivalent to the Lebesgue integral. As a Riemann-type integral, it is simpler to handle than the Lebesgue integral. Further, his integral does not involve concepts such as  $\sigma$ -algebras and measures. Several extensions of the McShane integral had been done. Gordon extended the definition to Banach-valued functions. Recently, Canoy also extended the definitions to functions with values in a ranked countably normed spaces.

In this study, we defined the McShane integral for functions with values in a topological vector space (TVS). Among others, this study generated results concerning the Cauchy test for integrability, integrability of the continuous functions, linearity of the integral, integrability on a subinterval, and additive property on subintervals.

Furthermore, since Banach spaces are topological spaces, this study showed that the TVS version and the Banach version of the McShane integral are indeed equivalent whenever the space under consideration is Banach space.

**Keywords:** topological, vector, Banach, McShane, integral, function



**CMPSD No. 22      WHICH DISCONNECTED GRAPHS POSSESS  
THE EULERIAN PROPERTY  $\pi$  ?**

**Sergio R. Canoy Jr.**

Department of Mathematics, College of Science and Mathematics  
MSU-Iligan Institute of Technology, 9200 Iligan City

Let  $G$  be a simple graph with nonempty edge-set. The line graph of  $G$ , denoted by  $L(G)$ , is the graph whose vertices are the edges of  $G$  and where two vertices of  $L(G)$  are adjacent whenever the corresponding edges have a common vertex in  $G$ . The graphs denoted by  $L^2(G)$  and  $L^3(G)$  are the line graphs of  $L(G)$  and  $L^2(G)$ , respectively. We say that a graph  $G$  is Eulerian if it has a spanning closed walk that traverses each edge of  $G$  exactly once. A simple graph  $G$  possesses the Eulerian property  $\pi$  if  $L^3(G)$  is Eulerian but  $L^2(G)$  is not.

For simple connected graphs, Uy showed that a graph possesses property  $\pi$  if and only if  $G$  is a path of order 4. Apparently, such a result for connected graphs does not hold for disconnected graphs. Thus, an interesting and natural question to ask is: Which disconnected graphs possess the Eulerian property  $\pi$ ? This research study aims to give an explicit answer to the question being posed. Specifically, we shall characterize all graphs  $G$  which carry property  $\pi$ , that is, those disconnected graphs  $G$  such that  $L^3(G)$  is Eulerian but  $L^2(G)$  is not.

As main result of the paper, the following characterization was obtained:

(\*) Let  $G$  be a disconnected graph with  $k+1$  components ( $k \geq 1$ ). Then  $G$  possesses the Eulerian property  $\pi$  if and only if  $G$  is equal (isomorphic) to one of the following graphs:

- (a)  $P_1 P_{s(1)} \dots P_{s(k)}$ , where  $1 \leq s(i) \leq 3$  for all  $i = 1, 2, \dots, k$ ;
- (b)  $C_n P_{s(1)} \dots P_{s(k)}$ , where  $1 \leq s(i) \leq 3$  for all  $i = 1, 2, \dots, k$  and at least one component is  $P_{s(i)} = P_3$ ; and
- (c)  $H P_{s(1)} \dots P_{s(k)}$ , where  $1 \leq s(i) \leq 3$  for all  $i = 1, 2, \dots, k$ ,  $H$  is of order at least 4, the degrees of the vertices of  $L(H)$  are of the same parity, and at least one  $P_{s(i)} = P_3$ .

**Keywords:** graph, disconnected, component, line graph, Eulerian

**CMPSD No. 23 ON THE EXISTENCE OF NON-ASSOCIATIVE  
FLEXIBLE DIVISION ALGEBRAS OF DIMENSION  $n=10$**

**Alexander S. Carrascal**

ECE Department, College of Engineering  
Polytechnic University of the Philippines, Sta. Mesa, Manila

An algebra  $A$  is a division algebra if given  $a, b \in A$  with  $ab = 0$ , then either  $a = 0$  or  $b = 0$ , i.e.,  $A$  has no zero divisors. The real numbers  $R$ , the complex numbers  $C$ , and the quaternions  $H$  exhaust all the associative division algebras over the real numbers (Frobenius, 1878). If the associativity requirement is dropped, the only additional division algebra over the real numbers is the octonions  $O$  (Boott-Milnor, 1957). The dimensions of these algebras are 1, 2, 4, and 8, respectively. Using the Cayley-Dickson process, the quaternions can be obtained from the complex numbers and the octonions from the quaternions. Subsequent application of this doubling process will result to higher-dimensional algebras that has zero divisors and hence not division algebras.  $R, C, H$ , and  $O$  are the only normed division algebras (Hurwitz, 1898). Moreover, they are the only alternative division algebras (Zorn, 1930). Although they are not the only division algebras, it was independently proved by Kervaire and Bott-Milnor (1958) that all division algebras have dimension 1, 2, 4, or 8. However, this paper will show that there exist 10-dimensional non-associative division algebras with multiplicative inverses and containing  $R, C$ , and  $H$  as its sub-algebras. Moreover, embedded in this algebra is a loop that has inverse property, flexible and alternative.

**Keywords:** Alternatively, flexibility property, inverse property, non-associativity, norm, division, algebra, zero divisors

**CMPSD No. 24 NON-ASSOCIATIVE FINITE LOOPS: POSSIBLE  
APPLICATIONS IN THEORETICAL PHYSICS**

**Raoul E. Cawagas**

SciTech R&D Center  
Polytechnic University of the Philippines, Sta. Mesa, Manila

It has been well noted that many physical systems have symmetries that are naturally described by associative mathematical structures like groups. Thus, the theories of atomic structure and of elementary particles make use of several group theoretic ideas in their mathematical formulations.

So far, non-associative mathematical structures like finite loops and quasigroups have played a limited role on science. However, such structures are beginning to show

great promise in formulating some of the most difficult problems of contemporary physics particularly in the study of elementary particles (quarks, string theory, unified field theories, etc.). The main "point of entry" of such non-associative structures in physics has been through what is known as the octonions (or Cayley numbers) which is the only non-associative real division algebra. The octonion units form a non-associative finite inverted loop of order 16 that is embedded in the octonion algebra. This algebra is now being used in such fields as quantum electrodynamics and related theories.

Lately, several classes of finite loops of small order have attracted the attention of certain theoretical physicists. These are the non-associative loops of orders 5 and 6, which have been found to define loop algebras that satisfy the Jacobi identity. Such algebras are also called Lie Algebras and these are known to be very useful in formulating physical theories.

Two of the loops in question are  $(L_5, *)$  of order 6 which we have been studying in connection with our program to develop the theory of Non-associative Finite Invertible Loops (NAFILS). Our analysis says that the loops  $(L_5, *)$  and  $(L_6, *)$  are the first members of two families (the ODD and EVEN families) of NAFILS. In particular,  $(L_5, *)$  is a non-abelian simple NAFIL while  $(L_6, *)$  is an abelian simple NAFIL. These two loops have interesting structures that are being considered as challenges for possible applications in physics. This paper aims to present our analysis of the structure of these interesting loops.

**Keywords:** finite loops, non-associative, Jacobi identity, Lie algebra, NAFILS, particle physics

## CMPSD No. 25      CHARACTERIZATION OF NAFIL LOOPS OF ORDERS 5, 6, AND 7 (ABELIAN)

Raoul E. Cawagas and Deana Laura Banatin

SciTech R&D Center  
Polytechnic University of the Philippines, Sta. Mesa, Manila

This paper deals with the characterization of non-associative finite invertible loops (NAFIL) of small order  $n=5, 6,$  and  $7$  (abelian). In particular, it corrects and completes the results of an earlier attempt to characterize these loops using the software FINITAS.

In a previous study done at PUP in 1996, all non-isomorphic NAFIL loops of orders  $n = 5, 6,$  and  $7$  (abelian) were determined using the program ICONSTRUCT. These loops were characterized using Version 1.0 of the software FINITAS but the results were incomplete. Because of several problems encountered in this initial study, we undertook a program to validate and complete the determination and characterization of these loops.

Accordingly, we again determined in 1999 all non-isomorphic NAFIL loops of orders  $n = 5, 6,$  and  $7$  using a more powerful software system (SEM-SATO) in collaboration with Prof. H. Zhang of the University of Iowa. This new determination validated the results obtained by ICONSTRACT and at the same time completed the generation of all non-abelian NAFILs of order  $n = 7$ . Having validated the generated NAFILs, we then characterized these loops again in 2001 using Version 1.1X of FINITAS. This updated version of FINITAS has vastly greater analytical capabilities that enabled us, finally, to sufficiently characterize all NAFIL loops of orders  $n = 5, 6,$  and  $7$  (abelian).

**Keywords:** NAFIL loops, non-isomorphic characterization, FINITAS

## CMPSD No. 26 CHARACTERIZATION OF PLAIN NAFIL LOOPS OF ORDER 7

**Renilda S. Layno**

SciTech R&D Center  
Polytechnic University of the Philippines, Sta. Mesa, Manila

In a previous study done at PUP in 2001, all non-isomorphic NAFIL loops of order  $n = 7$  were determined using a powerful software system (SEM-SATO) in collaboration with Prof. H. Zhang of the University of Iowa. This new determination completed the generation of all non-abelian NAFILs of order  $7$ , which were not completely determined in an earlier study in 1999 using the program CONSTRUCT.

Having generated all NAFILs of order  $7$ , we determined in 2001 the loops of this order with only one (1) self-inverse element. In particular, we were interested in those loops with no non-trivial subsystems called *plain* (or non-composite). The result of this study showed that out of 681 NAFIL loops of order  $7$  with one self-inverse element, 646 are *plain* while 35 are composite.

Type of NAFIL	Total Number	No. of Plain	No. of Composite
Abelian	16	8 (all w/prop)	8 (all w/prop)
Non-abelian	665	638 (8 w/prop)	27 (22 w/prop)
Total	681	646	35

This paper deals with the characterization of the 646 *plain* NAFIL loops (8 abelian and 638 non-abelian) of order  $7$ . This characterization involved determination of the

basic properties of these loops using the latest version of the software *FINITAS*. Using a characterization scheme developed in a previous study, we organized the data and showed that these loops can be *sufficiently characterized* in terms of their basic properties.

**Keywords:** *NAFIL*, loops, non-isomorphic, characterization, *FINITAS*, non-isomorphic

### CMPSD No. 27 CONDUCTIVITY OF THE SEMICONDUCTING BF<sub>4</sub><sup>-</sup> - DOPE POLYTHIOPHENE FILM

Editha P. Jacosalem<sup>1</sup>, Angelina M. Bacala<sup>1</sup>, L.D. Pamatong<sup>1</sup>, Reynaldo M. Vequizo<sup>1</sup>, M. Munoz<sup>1</sup>, R.L. Reserva<sup>1</sup>, E. Gooe<sup>1</sup>, B. Entera<sup>1</sup>, Y. Sasaki<sup>2</sup>, K. Yamada<sup>2</sup>, K. Fujiwara<sup>2</sup>, N. Nakajima<sup>2</sup>, H. Miyata<sup>2</sup>, A. Kimura<sup>3</sup> and M. Shirai<sup>4</sup>

<sup>1</sup>Department of Physics, MSU-Iligan Institute of Technology (MSU-IIT)  
Andres Bonifacio Avenue, 9200 Iligan City

<sup>2</sup>Department of Physics, Niigata University, Ikarashi Ni-nocho, Niigata, Japan

<sup>3</sup>Osaka Institute of Technology, Osaka, Japan

<sup>4</sup>Niihama National College of Technology, Japan

Organic conducting polymers like polythiophene (PT) and its derivatives have gained much attention nowadays due to their promising applications both fundamentally and technologically. It is the controllable conductivity of these polymers that interest most of the researchers. The characteristic behavior of the resistivity and conductivity of the electrochemically prepared PT film sample is investigated in this paper.

Tetrafluoroborate (BF<sub>4</sub><sup>-</sup>) - doped polythiophene film sample was synthesized electrochemically in a two - electrode polymerization cell. The Indium Tin Oxide (ITO) and platinum electrodes were used in the beaker type polymerization cell as the working and the counter electrodes respectively. The electrolyte used was 1.575 M thiophene/ 1.800 M LiBF<sub>4</sub> in dehydrated acetonitrile (MeCN). The polymerization voltage was set at 20.0 volts at -2°C. The stamp voltage, time and the current during polymerization accompanied with doping as well as the dedoping of the PT polymer were recorded. The oxygen concentration in the cell was monitored. The electropolymerization was carried out under nitrogen gas atmosphere. The temperature dependence of the conductivity was also performed. At room temperature, the conductivity was measured employing the standard four-probe technique.

The electropolymerization yielded a compact and non-powdery greenish PT film sample. This 284 micron - thick green film can easily be peeled off from the indium tin oxide (ITO) substrate. The room temperature conductivity along the surface of the film was found to be  $3.0 \times 10^{-5}$  S / cm. This conductivity signifies the semiconducting property

of this film. The remarkable linear temperature dependence of the conductivity was observed. This dependence obeys  $T^{-n}$  with  $n = 1$  and suggests two - dimensional variable - range hopping of the conduction mechanism in the polymeric film

**Keywords:** electropolymerization, polythiophene, four-probe technique

### **CMPSD No. 28 THE RADIATION DETECTION CHARACTERISTICS OF THE SEMICONDUCTING POLYTHIOPHENE FILM**

**Reynaldo M. Vequizo<sup>1</sup>, Angelina M. Bacala<sup>1</sup>, Y. Sasaki<sup>2</sup>, K. Yamada<sup>2</sup>, K. Fujiwara<sup>2</sup>, N. Nakajima<sup>2</sup>, H. Miyata<sup>2</sup>, A. Kimura<sup>3</sup> and M. Shirai<sup>4</sup>**

<sup>1</sup>Department of Physics, MSU-Iligan Institute of Technology (MSU-IIT)  
Andres Bonifacio Avenue, 9200 Iligan City

<sup>2</sup>Department of Physics, Niigata University, Ikarashi Ni-nocho, Niigata, Japan

<sup>3</sup>Osaka Institute of Technology, Osaka, Japan

<sup>4</sup>Niihama National College of Technology, Japan

Since the discovery of the conducting polyacetylene (PA) with the introduction of the appropriate dopant, scientific researches on the fundamental and practical applications of organic conducting polymer systems like polythiophene, have gained considerable interests to the scientific community. In spite of the fact that the promising applications of PT are widely studied nowadays, there are only few reports on the fabrication of radiation sensors. The present study mainly focuses on the photon response of the polymeric film sample of PT which is electrochemically polymerized in an acetonitrile containing dopant anion polymerization cell. The characteristics radiation detection of this film was specifically investigated.

Polythiophene film sample was prepared via anodic electropolymerization of thiophene in an indium tin oxide (ITO) evaporated glass substrate inside a two-electrode polymerization cell set at 20 volts and -2.0°C. The already  $BF_4^-$  doped PT film was dedoped potentiostatically at -30 volts at the same temperature. A strip of the PT film sample was cut, and the fabrication of a radiation sensor sample out of this strip followed. As initial characterization, the sensor is electrically characterized by performing the Current-Voltage (I-V) measurement. The signal was then observed from the oscilloscope as the sensor was irradiated with Nd:YAG Laser. The final systematic characterization was done via on-line data acquisition using Nuclear Instrument Module (NIM) and the Computer Automated Measurement And Control (CAMAC) modules to perform analog-to-digital conversion (ADC) test.

The PT sensor exhibited ohmic behavior at room temperature when I-V measurement was done. The evident signals from the PT sensor when irradiated with Nd:YAG Laser could be observed. These signals showed a rise time that ranges from

$10^{-9}$  -  $10^{-6}$  seconds. These were signals that could be processed for sensor calibration. At room temperature, this sensor showed a characteristic resolution of less than 25% when illuminated with Nd:YAG laser operating at 532 nm wavelength, 5Hz frequency and low intensity. The evident plateau exhibited by the signal-to-noise  $S/N$  ratio vs Bias Voltage curve, indicates the stable charge collection during irradiation. It has an operating voltage of 325 Volts as a radiation sensor.

**Keywords:** organic polymers, polythiophene, electropolymerization, NIM & CAMAC, ADC

### **CMPSD No. 29 SUPERCONDUCTING PROPERTIES OF LEAD-DOPED BSCCO GLASS CERAMICS**

Shirley Tiong-Palisoc<sup>1</sup> P.P. Mendoza<sup>2</sup>, S. S. Fontanilla<sup>1</sup>,  
M.V. Beltran<sup>1</sup>, V.V. Villanueva<sup>1</sup>

<sup>1</sup> Physics Department, De La Salle University, Taft Avenue, 2401 Manila

<sup>2</sup> Holy Angels University, Angeles City, Pampanga

This paper reports on the preparation of high  $T_c$  BPbSCCO superconducting ceramics prepared by melt-quench-anneal technique as well as the growth of the high  $T_c$  superconducting phase of the BPbSCCO ceramics in a certain range of composition.

Lead doped BSCCO ceramics with stoichiometric composition of  $\text{Bi}_{1-x}\text{Pb}_x\text{Sr}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_y$  with  $n = 2.0, 2.5, 3.0$  and  $3.5$  are investigated in this study. The lead doped BSCCO samples are characterized by X-ray Diffractometry (XRD), and Scanning Electron Microscopy (SEM). The temperature dependence of resistance of some samples are also measured by means of  $r$ - $T$  (resistivity vs temperature) and  $c$ - $T$  (magnetic susceptibility vs temperature) tests.

The XRD results show that the peaks attributed to the high- $T_c$  phase changed in its intensity as  $n$  is increased, wherein it coincided with increased Ca and Cu which facilitated the growth of the high- $T_c$  phase.

$T_c$  results ( $r$ - $T$  and  $c$ - $T$  measurements) indicate that an excess of Cu element which is inferred as a deviation from the nominal composition of the high  $T_c$  phase caused a degradation of the superconducting property although the high  $T_c$  phase formation is enhanced as seen from the XRD results.

SEM analysis show that the sample for  $n = 3.0$  having the higher  $T_c$  of 106K has advanced crystal growth as compared to the samples for  $n = 2.0, 2.5$  and  $3.5$ . The crystallites are more pronounced in  $n = 3.0$  as compared to the other samples. The plate-like grains in the samples for  $n = 2.5$  and  $3.5$  are more dense and seem like they just nucleated. This may explain the low  $T_c$  results for  $n = 2.5$  and  $3.5$ .

**Keywords:** superconducting ceramic, SEM, XRD

**CMPSD No. 30 AC MAGNETIC SUSCEPTIBILITY OF YBCO:  
FREQUENCY AND MAGNETIC FIELD DEPENDENCE**

**Maria Veronica G. Sibayan and Roland V. Sarmago**

Condensed Matter Physics Laboratory, National Institute of Physics  
University of the Philippines Diliman, 1101 Quezon City

Studies on linear and nonlinear AC susceptibility provide much insight into the loss mechanism and flux dynamics of high-temperature superconductors (HTS). The imaginary part of the complex AC susceptibility in particular is a direct measure of AC losses, the study which provides information on the critical state of the superconducting material. In the present paper, the imaginary susceptibility of YBCO was investigated by doing AC magnetic susceptibility measurements using a Mutual Inductance Bridge (MIB) setup on sintered YBCO for various applied magnetic fields ranging from 0.2mT to 2.0mT and excitation frequencies ranging from 110Hz to 1800Hz.

The out-of-phase signal obtained has two distinctly observed peaks. A sharp peak was found in the vicinity of the critical temperature  $T_c$  and is observed to sharpen as it shifts to higher temperatures with increasing excitation frequency. It sharpens but remains fixed in position in temperature with increasing applied magnetic field. This peak near  $T_c$  is attributed to the hysteric behavior of the superconductor and is expected to be frequency-dependent.

A broad peak was found at a lower temperature and is observed to broaden as it shifts to lower temperature with increasing applied magnetic field. It sharpens but remains fixed in position in temperature with increasing frequency. This peak is attributed to energy loss due to intergranular shielding currents. The shifting of this peak to lower temperatures is attributed to the increased flux threading in the porous regions of the sample brought by the increase in the applied magnetic field. It is not expected to be frequency-dependent.

The results obtained verify that the hysteresis loss peak and the intergranular loss peak are driven by different mechanisms, as they respond differently on frequency and field. This implies that one should be able to obtain two peaks in the imaginary susceptibility of a granular superconductor.

**Keywords:** YBCO, hysteresis loss peak, intergranular loss peak, AC magnetic susceptibility, superconductor



**CMPSD No. 31 EFFECTS OF SINTERING TEMPERATURE,  
AMBIENT ATMOSPHERE AND TIME ON THE MICROSTRUCTURE  
AND SUPERCONDUCTIVITY OF BULK  $MgB_2$**

**Margie P. Olbinado, Jose D. Guerra and Roland V. Sarmago**

Condensed Matter Physics Laboratory, National Institute of Physics  
University of the Philippines Diliman, 1101 Quezon City

We have previously shown that compaction and sintering of commercial magnesium diboride ( $MgB_2$ ) powder at temperatures below  $800^\circ C$  is promising for preparation of bulk superconducting  $MgB_2$ . In this work, we report on the effects of sintering temperature, ambient atmosphere and time on the superconductivity and microstructure of bulk  $MgB_2$ . Superconductivity of the pellets were determined from dc resistivity and ac magnetic susceptibility measurements while the microstructure was derived from scanning electron microscopy (SEM). For both Ar and vacuum atmosphere, we found that increasing the sintering temperature enhances the superconductivity of the pellets. This is manifested by a higher superconducting transition temperature,  $T_c$ , and a narrower transition width,  $\Delta T$ . The optimum sintering temperature being  $750^\circ C$ . However,  $T_c$  is higher and  $\Delta T$  is narrower for pellets sintered under Ar atmosphere. On the other hand, increasing the sintering time reduces  $T_c$  and broadens  $\Delta T$ . These effects on the superconductivity were closely related to the changes on the surface morphology of the pellets as observed from SEM.

**Keywords:** magnesium diboride, sintering temperature, sintering atmosphere, sintering time

**CMPSD No. 32 SIMULTANEOUS MEASUREMENTS  
OF COSMIC RAY FLUX**

**Rosario L. Reserva<sup>1</sup>, Angelina M. Bacala<sup>1</sup>, M.C. Garcia<sup>2</sup>,  
R.M. De Asis<sup>2</sup> and E.J. Jacosalem<sup>1</sup>**

<sup>1</sup>Department of Physics, MSU-Iligan Institute of Technology (MSU-IIT)  
Andres Bonifacio Avenue, 9200 Iligan City

<sup>2</sup>Ateneo de Zamboanga University, Zamboanga City

Cosmic rays are highly energetic particles of extra-terrestrial origins. These form part of the natural radioactivity experienced by humans and recent experiments have shown that cosmic rays also affect the subtle performance of electronic logic memories in computers.

Real-time measurements of cosmic ray flux at sea level in Iligan City and

Zamboanga City are simultaneously taken in preparation for a Mindanao-wide mapping of cosmic ray flux. The cosmic ray detector used in each location is a vertical stack of two 8" x 8" x 1/2" plastic scintillators, 100 cm apart, each optically coupled to a 2" diameter photomultiplier tube. The anode signals from each plastic scintillator detector will pass through nuclear instrumentation modules (NIM) among which are: the discriminator, variable delay, scaler and coincidence module. Measurements are taken at these places simultaneously for a period of several months and for several hours each during the day and night to observe any nighttime and daytime variations in the cosmic ray flux. Collected data are analyzed using standard statistical methods. Results are then compared with the first measurement of cosmic ray flux at sea level in Iligan City which was done by E. Ninofranco in 1999. Using a similar array of plastic scintillator detectors and NIM electronic module assembly. Ninofranco measured the average cosmic ray flux to be equal to  $10.52 \pm 0.43$  particles/min and further noted that this was the same during day or night. His measurements were shown to be consistent with internationally-accepted values and also consistent with Monte Carlo simulation of the experiment.

It has been predicted that at sea level the cosmic ray flux is constant at fixed latitudes. A Third World Academy of Sciences funding is being awaited to start the mapping of the cosmic ray flux throughout the whole island of Mindanao by simultaneous measurements of cosmic radiation at 5 different locations of the island.

**Keywords:** cosmic ray flux, scintillation detectors, NIM instrumentation modules, Monte Carlo simulation

### **CMPSD No. 33 STUDY ON THE CHAMBER PERFORMANCE OF THE JLC-CDC BABY CHAMBER**

**Hermogenes C. Gooe Jr.<sup>1</sup>, D. C. Arogancia<sup>1</sup>, J. B. Magallanes<sup>1</sup>,  
Angelina M. Bacala<sup>1</sup>, K. Fujii<sup>2</sup>, JLC-CDC SUBGROUP**

<sup>1</sup>Computational High Energy Physics Laboratory,

Department of Physics, MSU- Iligan Institute of Technology, 9200 Iligan City

<sup>2</sup>Institute of Particle and Nuclear Science, KEK, Tsukuba, Japan

JLC (Joint Linear Collider) is a proposed  $e^+e^-$  linear collider to be built in Japan, which is expected to discover and determine the properties of the Higgs boson. One of its components is the Central Drift Chamber (CDC), which will determine the information of the tracked particles. A small test chamber called the baby chamber was fabricated with the same jet cell structure as the 4.6 m-long test drift chamber, which is constructed with the current design of the CDC, in order to carry out beam tests on basic chamber performance including efficiency, spatial resolution and two-track separation capability. A software has been developed to analyze the beam test data to study the performance of this chamber by optimizing chamber parameters to obtain maximum performance. The data used in this study was taken during the beam test using the electron-positron pairs

produced by bremsstrahlung photons from the internal target of REFER (Relativistic Electron Facility for Education and Researches) in Hiroshima University, Japan. By computer analyses of the beam test data, the obtain wire efficiency of above 96% over the entire drift length of 5 cm. Also, the spatial resolution of the central sense wire of the first cell is below 85  $\mu$ m when the drift length is less than 3.0 cm. These results are in good agreement with the result obtained using the 4.6 m-long test drift chamber. In studying two-track separation capability, the two-track separation efficiency is plotted against two-hit distance and we found out that the test chamber can separate two-tracks which are separated by 2mm or less by 70%. Further fine tuning of parameters must be done in order to achieve the performance goals of the drift chamber.

**Keywords:** Higgs boson, Joint Linear Collider (JLC), Central Drift Chamber (CDC), baby chamber, JLC Study Framework (JSF), efficiency, spatial resolution, two-track separation, drift length, two-hit distance

**CMPSD No. 34      ENHANCEMENT OF THE  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10,d}$  PHASE  
IN Bi-Sr-Ca-Cu-O FILMS GROWN VIA LIQUID PHASE EPITAXY**

**Adrel Voltaire A. Cueto, L.J.D. Guerra, Ivan Ronald O. Ambanta  
and Roland V. Sarmagu**

Condensed Matter Physics Laboratory, National Institute of Physics  
University of the Philippines, Diliman, Quezon City

The successful growth of single phase  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10,d}$  (Bi2223) has never been demonstrated. Instead, inter-growth of the various Bi-Sr-Ca-Cu-O (BSCCO) phases is observed. In this work, the growth and annealing parameters needed to increase the volume fraction of the Bi2223 phase in BSCCO films is investigated. In particular, the composition of the melt and the annealing temperatures are varied while the volume fraction of Bi2223 is derived from high-resolution X-ray Diffraction (XRD). Surface morphology of the grown films was studied using Scanning Electron Microscope (SEM) while their superconductivity was confirmed through DC resistivity measurements. We found that the use of non-stoichiometric melts (with excess Ca and Cu atoms) increases the Bi2223 volume fraction. However, excess Sr atom in the melt is seen to decrease the Bi2223 volume fraction. Moreover, annealing the as-grown films at 840 °C to 860 °C is seen to further increase the volume fraction of Bi2223 as reported by other groups. From dc resistivity measurements, the transition attributed to the Bi2223 phase increases as the volume fraction of Bi2223 increases. These results indicate that excess Ca and Cu atoms are needed to induce Bi2223 phase formation.

**Keywords:** phase enhancement,  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10,d}$ , BSCCO, annealing

**CMPSD No. 35 GROWTH OF SINGLE-PHASE, C-AXIS ORIENTED  
Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8</sub> (Bi-2212) SUPERCONDUCTING THIN  
FILMS VIA LIQUID PHASE EPITAXY (LPE) FROM  
STOICHIOMETRIC AND NON-STOICHIOMETRIC MELTS**

**Ivan Ronald O. Ambanta, L.J.D. Guerra, Adrel Voltaire A. Cueto,  
M.P. Olbinado and Roland V. Sarmago**

Condensed Matter Physics Laboratory  
National Institute of Physics, College of Science  
University of the Philippines Diliman, 1101 Quezon City

The growth of high-quality superconducting thin films is necessary to develop superconducting devices. Although liquid phase epitaxial growth of Bi-2212 has been demonstrated, the growth of Bi-2212 films from non-stoichiometric melts has not been extensively pursued. In this work, we report on the successful growth of homogenous, single-phase, c-axis oriented Bi-2212 superconducting thin films via LPE from stoichiometric and non-stoichiometric melts on single crystalline magnesium oxide (MgO) and polycrystalline aluminum oxide (Al<sub>2</sub>O<sub>3</sub>) substrates. Preferential orientation and phase purity of the grown films were determined through high-resolution x-ray diffraction (XRD) while the surface morphology was obtained from scanning electron microscopy (SEM). DC resistivity measurements confirmed the superconductivity of the grown films with T<sub>c</sub> = 75-85 K. From XRD, we found that the as-grown films from stoichiometric melts had no preferential orientation but subsequent annealing at 840-860°C in oxygen (O<sub>2</sub>) atmosphere converted the non-(00l) peaks to (00l) peaks. For the as-grown films from non-stoichiometric melts, XRD shows both Bi-2201 and Bi-2212 peaks but annealing at 840-860°C in O<sub>2</sub> converted the Bi-2201 peaks to Bi-2212 peaks with some increase in XRD peak intensity. SEM shows complete coverage of the substrate and the granular nature of the films. These results show excess Ca and Cu atoms contribute to Bi-2212 growth.

**Keywords:** Liquid phase epitaxy, Bi-2212 thin films, superconductivity

**CMPSD No. 36 MAGNETIC RESPONSE OF GRANULAR  
HIGH-TC SUPERCONDUCTORS**

**Bess G. Singidas and Roland V. Sarmago**

Condensed Matter Physics Laboratory  
National Institute of Physics, College of Science  
University of the Philippines Diliman, 1101 Quezon City

The magnetization of a granular superconductor was examined by approximating