CHEMICAL, MATHEMATICAL AND PHYSICAL SCIENCES

CMPS - 01

DISCRIMINATION OF PHILIPPINE COFFEE BEANS USING AN ELECTRONIC NOSE SYSTEM BASED ON POLYMER-COATED PIEZOELECTRIC QUARTZ CRYSTAL

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Electronic nose (EN) generates an electrical signal in the presence of a substance causing aroma. In this study, the feasibility of a fabricated EN based on polymer-coated piezoelectric quartz crystals (PQC) was investigated for the discrimination of the different coffee varieties in the Philippines (i.e. Arabica, Robusta, Excelsa and Liberica). The EN system that was employed was based on PQC coated with six sensing elements of different polarities [polyethylene glycol (PEG), polyvinylchloride (PVC), Silica (PVC/Silica), Cat-Ex (PVC/CatEx)], polymethylacrylate (PVC/PMAA) and Fluorosil (PVC/Fluor). Using the optimized conditions, coffee samples were sealed separately in the suitable vial and the headspace gas was pumped through the EN system using nitrogen gas. The gas phase detection was based on the corresponding change on the frequency of the crystal. Distinct radar plot quality profiles were obtained for each variety. Chemometric analysis of the responses from 48 different coffee samples using the EN was carried out using principal component analysis (PCA) and cluster analysis (CA). PCA and CA were applied to classify and to quantify how coffee samples are close to each other. The developed group of sensors was then able to categorize the different coffee varieties.

Keywords: piezoelectric quartz crystal; electronic nose; chemometric analysis, principal component analysis, cluster analysis

CMPS - 02

ELECTROCHEMICAL PROPERTIES OF PtRuSn TERNARY ELECTROCATALYST DISPERSED ON POLY(3,4-ETHYLENEDIOXYTHIOPHENE) (PEDOT) FOR FUEL CELL APPLICATION

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Fuel cells have been considered as an effective alternative energy source due to its efficient energy conversion and low pollutant emissions. Therefore, improvement in alcohol oxidation is important in fuel cell technology and this can be achieved by developing modified platinum as electrocatalyst. Electrocatalytic oxidation of ethanol in acidic medium was studied using PtRuSn-PEDOT-modified polycrystalline and (111)-oriented single crystal electrodes of Au and Pt electrodes. In this study, potential cycling from –400 to 850 mV (vs. Ag/AgCl) was employed in depositing the Pt particles. Spontaneous deposition of Ru at 120 seconds with reduction at a constant potential (50 mV) was observed to be the most effective method in depositing Ru. This method was also used to deposit Sn particles for the preparation of PtRuSn ternary electrocatalyst. It was observed that 1 mM exhibits the most effective concentration towards ethanol oxidation. The developed ternary electrocatalysts had shown higher electrocatalytic activity by 15.00% – 21.22% than the binary catalysts. The same surface modification methods were employed on Au(111) and Pt(111) single crystal electrodes. It was observed that (111) single crystal substrates exhibit higher electrocatalytic activity by 10.69% (for Au(111)) and 72.63% (for Pt(111)) than their polycrystalline counterparts. As revealed by SEM, PEDOT electrochemically grown on the well-defined single crystal electrode surface was more ordered and smoother than on the polycrystalline substrate. This gave a better dispersion of the electrocatalysts on the PEDOT matrix, leading to more catalytic active sites.

Keywords: fuel cells, alcohol oxidation, electrocatalyst, cyclic voltammetry, spontaneous deposition

CMPS - 03

A HYBRID GAS SENSOR ARRAY FOR THE QUALITY ASSESSMENT OF VIRGIN COCONUT OILS

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A hybrid gas sensor system composed of seven chemiresistors based on thin conducting polymer (CHCP) films and nine polymer-coated piezoelectric quartz crystals (PPQC) were developed and utilized for assessing the quality of virgin coconut oil. The sensors were exposed to the headspace of samples of virgin coconut oil (VCO), refined, bleached and deodorized coconut oils (RBD), rancid VCO and flavored VCO. The response of the chemiresistor was measured using a bridge circuit operating in a deflection mode, and the response of the piezoelectric quartz crystals was measured using an instrumentation system involving an oscillator circuit and a frequency counter. The CHCP sensors displayed good reproducibility (rsd= 2.02% to 10.40%; n=6) and reversibility (rsd= 0.033% to 1.98%; n=3). At the same time, PPQC also exhibited good reproducibility (rsd= 3.54% to 6.28%; n=3) and reversibility (rsd=3.83% to 7.95%; n=3). Chemometric analysis of the data through principal component analysis (PCA) enabled a very good discrimination of VCO, RBD, rancid VCO and flavored VCO with a cumulative variance of 81.87%. This hybrid gas sensor system will be very useful in monitoring the quality of VCO products and will detect adulterated and fraudulent VCO products.

Keywords: hybrid sensor array, chemiresistor, piezoelectric quartz crystal, conducting polymers, VCO

CMPS - 04

FISH FRESHNESS ANALYSIS USING A POLYANILINE/ NYLON COMPOSITE-BASED CHEMIRESISTOR SENSOR

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Food safety assurance is an important factor in building confidence to consumers when choosing a particular product. In the fish sector, freshness of fish is placed into a great consideration in order to ensure the health and safety of the consumers, and to maintain the quality of their products. Trimethylamine (TMA), a volatile amine compound responsible for the pungent, fishy, ammonia like aroma in fish, is a typical marker for fish freshness detection. TMA is the toxic gas found after death of a fish. In previous studies, a series of inspections were performed to determine freshness of fish, but methods are ineffective and found to be time consuming.

In this study, a chemiresistor sensor based on polyaniline (PANI)/ nylon composite was developed for the headspace analysis of trimethylamine. The polymer composite was prepared by an *in situ* chemical oxidative polymerization of 0.4 M aniline with an equimolar amount of HCl onto a nylon membrane using 0.6 M ammonium peroxysulfate oxidant. The composite was mounted on a home-made assembly for resistivity measurement based on the four-point probe method. The assembly design allowed the membrane composite to be in contact with the headspace of the measurand system. The measured resistance varied with the TMA concentration, exhibiting a sensitivity of 14.05 mA/- log ppb TMA and linearity (r) of 0.975 at a dynamic concentration range of 10^{-9} to 10^{-6} ppb TMA. It is repeatable showing a COV of 7.8% for the 10^{-6} ppb sample cycled thrice. TMA in fish was detected on the 8th hour of exposure. This type of gas sensor is attractive because it provides a promising low-cost means to monitor TMA at RT.

Keywords: fish freshness, polyaniline/nylon composite, trimethylamine, chemiresistor, gas sensor

CMPS - 05

ELECTROCHEMICAL SYNTHESIS AND CORROSION PERFORMANCE OF POLYPYRROLE AND POLY(PYRROLE-CO-ANILINE) FILMS ON COPPER

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The cheapest and most commonly used metal to date is copper, which is highly prone to corrosion. However, copper is mostly used in highly corrosive environment, which degrades the metal's durability and costs money to multinational businesses. To protect metals, conducting polymers are one of the most promising materials.

In this study, the electropolymerization of polypyrrole and poly(pyrrole-co-aniline) on copper electrode was done with cyclic voltammetry. A 0.1M pyrrole (Py) in 0.1 M near neutral (pH 7.6) $Na_2C_2O_4$ solution was used and a potential window of -0.5 V to +1.8 V. For the preparation of poly(pyrrole-co-aniline), a 0.1 M monomer solution of 0.5 M pyrrole and 0.5 M aniline were used.

The corrosion protection properties of these polymers were studied using the open circuit potential (OCP) measurement in 3.5% NaCl (aq). PPy had the best corrosion protection properties, followed by poly(pyrrole-co-aniline). PPy showed responses going towards more positive potentials compared to the copolymer and bare copper upon immersion to saline solution, which is due to both the pseudo-layer of copper oxalate complexes formed on the copper surface before polymerization and the polymer coat synthesized on its surface. SEM micrographs showed that polypyrrole exhibited multiple layers synthesized on the surface of copper, which contributed to its efficiency on protecting copper from corrosion.

Keywords: polypyrrole, polyaniline, corrosion, open-circuit potential, votammetry

CMPS - 06

PREPARATION AND INVESTIGATION OF SPIN SELF ASSEMBLED MULTILAYER FILM OF POLY(3,4 ETHYLENEDIOXYTHIOPHENE):POLY(4 STYRENESULFONATE) AND POLY(ALYLAMINE HYDROCHLORIDE) AS ORGANIC LIGHT-EMITTING DIODE

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The preparation and characterization of thin-film materials is a dominant area of research. These films have found several applications as thin-film and field effect transistors, touch displays and electroluminescent devices such as organic light-emitting diodes. The organic light-emitting diode (OLED) has received a lot of attention because of its attractive features for display applications. This study aims to chemically prepare poly (3,4-ethylenedioxythiophene):poly (styrenesulfonate) (PEDOT:PSS) and fabricate a polymer multilayer film with poly(allylaminehydrochloride) (PAH) by spin self-assembly method and to investigate the properties of the multilayer film as OLED.

EDOT was polymerized with PSS using $FeCl_3$ oxidant with several monomer to oxidant molar ratios (1:1, 1:2.5, 1:5, 1:7.5), with the 1:7.5 ratio giving the highest yield of polymer. The optical absorptions of several PEDOT:PSS solutions (0.05, 1, 3 and 5% w/v) showed 3% w/v with the highest and most stable reading with absorption peaks at 325 nm and 750 indicative of PSS and 990 nm for the blue-colored PEDOT. The PAH/PEDOT:PSS solution was spin-coated (2500 rpm for 30s) to form a film on glass slide and indium tin oxide substrates (1.0 x 2.5 cm). The film coating with a total of 15 bilayers showed an increasing absorbance as bilayer increases. SEM and AFM micrographs of PEDOT:PSS showed relatively smooth surface The OLED characteristic of the multilayer film gave a current-voltage curve of a diode even if no light was emitted.

Keywords: OLED, PEDOT, LBL films, spin self-assembly, AFM, SEM

CMPS - 07

FABRICATION AND CHARACTERIZATION OF SPIN-ASSISTED AND DIP-COATED PEDOT:PSS AND POLY(DIALLYDIMETHYLAMMONIUM CHLORIDE) NANOFILMS FOR ORGANIC LIGT-EMITTING DIODE

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Organic light emitting diodes (OLED) have extended its domain of applications in the area of flat panel displays due to their potential properties, brightness efficiency, extended lifetime and low production cost. The study aims to prepare and characterize nanofilms of Poly (3,4-ethylenedioxythiophene):Poly (styrenesulfonate) (PEDOT:PSS) and Poly (diallyldimethylammonium chloride) (PDADMAC) for the fabrication of an OLED.

EDOT:PSS was chemically polymerized using $(NH_4)_2S_2O_8$ oxidant and $FeCl_3$ catalyst. Absorbances of different solutions of synthesized PEDOT:PSS were determined using a UV-visible spectrophotometer. The glass slides and ITO-coated slides (10x20 mm) substrates were degreased and functionalized. In dip-coating, the treated substrate was then initially immersed in 0.01M PDADMAC solution for 15 min, followed by immersion in 3% (w/v) PEDOT:PSS solution. In spin-coating, PDADMAC and PEDOT:PSS were deposited alternately on the substrate with spin speed of 2500 rpm for 30 sec. The cycles for two techniques were repeated until 10 bilayers were achieved.

Each bilayer exhibited absorbance peaks at 370, 560 and 850 nm due the dark blue PEDOT. The SEM micrographs of PEDOT:PSS surfaces revealed globular structures. Atomic force micrographs showed average roughness of 1.000 nm and 14.697 nm, for spin-assisted and dip-coated films, respectively. An OLED was fabricated using PEDOT:PSS/PDADMAC films as the hole transport layer. The current-voltage graph of prepared OLED showed a diode characteristic.

Keywords: OLED, PEDOT, layer-by-layer films, spin-coated, dip-coated

CMPS - 08

RAPID SYNTHESIS UNDER MILD CONDITIONS OF AN ACRYLIC DIAMIDE N, N, N', N'T ETRABUTYLPHTHALAMIDE, APOTENTIAL ANTIMICROBIAL AGENT

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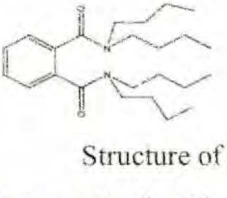
The amide functional group is a common feature in both small and complex synthetic or natural molecules. It is one of the most significant functional groups of organic molecules in terms of medicinal use. Medicinal Chemistry database showed that approximately 25% of known drugs contain this carboxamide group. The synthesis of acyclic diamide, N, N, N', N' – tetrabutylphthalamide, by the condensation with phthalic anhydride in dioxane of dibutylamine proved to be highly efficient. A product yield of 85% was obtained under mild conditions (6-hour reaction time at 27ÚC). The product was recrystallized in acetonitrile. The successful synthesis was confirmed through spectroscopic techniques such as infrared, nuclear magnetic resonance and mass spectroscopy. The purified product was tested for antimicrobial activity against *Escherichia coli*, *Staphylococcus aureus*, *Candida albicans* and *Aspergillus niger*. Chlorampenicol and clotrimazole were used as positive controls. The acyclic diamide exhibited antimicrobial activity with an antimicrobial index of 0.1 against *Escherichia coli*, 0.3 against *Staphylococcus aureus* and 0.2 against *Candida albicans*. No inhibition activity against *Aspergillus niger* was observed.



Structure of N, N, N', N' –tetrabutylphthalamide

Keywords: acyclic diamide, medicinal chemistry, condensation reaction, antimicrobial agent, antimicrobial index

CMPS - 09

EFFECT OF PRETREATMENT ON THE STRUCTURE AND CATALYTIC PROPERTIES OF RICE HULL-DERIVED ZEOLITES

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Rice hull was used as raw material for zeolite synthesis. It was pretreated with water and 1 M HCl before ashing at 600 °C in a muffle furnace for 3 hours. Purity of the rice hull ashes was verified by their percent carbon content. Characterization of the zeolites were done using electron dispersive X-ray (EDX), scanning electron microscopy (SEM) and X-ray diffraction (XRD) spectroscopy.

The rice hull pretreated with water had 21:16 (Si:Al) framework ratio while that pretreated with acid had 23:17 (Si:Al) which could mean that the Si-Al framework ratio of the samples could be about 1.3:1. SEM scans at 7500x magnification revealed that zeolites derived from rice hull ash pretreated with water had bigger pore sizes (2 μm) than those of acid-washed (1μm) diameter.

The catalytic properties of the prepared zeolites were determined by spiking a water sample with 69.0 ppm of NO_3^- solution (the maximum tolerable limit of nitrate in water), loading it with 0.2 g zeolite per liter of solution and aliquots analyzed after 2, 3 and 4 hours. The zeolite derived from water-pretreated ash removed nitrate in water (99.11%) and is not significantly different from that obtained from acid-pretreated ash (99.26%) after 4 hours. For comparison, commercial-grade zeolite was tested and was found to remove only 98.77% nitrate and is significantly different from the pretreated ones. Hence, pretreatment of the rice hull has an effect on the structure and catalytic properties of rice hull-derived zeolites.

Since water-pretreatment and acid-pretreatment yield zeolites that relatively remove nitrates in water, it is recommended that the former be employed for rice hull pretreatment. Study must be done also to determine the possibility of regenerating the zeolite after its use to remove nitrate.

Keywords: rice hull-derived, pretreatment, zeolites, catalytic, nitrate

CMPS - 10

SYNTHESIS OF GLYCEROL-CROSSLINKED POLY(METHYL METHACRYLATE) MICROPARTICLES FOR THE CONTROLLED DELIVERY OF MOSQUITO REPELLENT

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Crosslinked polymers can act as controlled release device to serve as sustained release source of mosquito repellant for a long period of time. One such polymer is poly(methylmethacrylate)(PMMA). However, being relatively hydrophobic it shows limited swelling in amphiphilic and polar solvents and hence limits its encapsulation and release application. This can be remedied by the use of a more hydrophilic moiety in the polymer network such as glycerol which is highly hydrophilic due to the presence of three hydroxyl (–OH) groups. Hence the research focused on the fabrication of glycerol crosslinked poly(methyl methacrylate) (GXPMMA) nanoparticles that can be used for the controlled release of mosquito repellent DEET(N,N-diethyl-m-toluamide). GXPMMA was synthesized by polymerization and crosslinking MMA with glycerol in one step in the presence of biocatalyst Novozyme 425, intiator benzoyl peroxide in toluene. It was observed that increase in reaction temperature from 50 to 70 °C, and decrease in the amount of toluene resulted in the formation of the product in shorter period of time. GXPMMA showed maximum swelling in amphiphilic solvent acetone. GXPMMA was converted into nanoparticles of size 200 nm by nanoprecipitation technique. DEET was incorporated into nanoparticles by dispersing the particles in acetone containing DEET. It was observed that when the nanoparticles: DEET was in the ratio of 1:0.5, 80% of free DEET got incorporated in 4 h. DEET was released at a controlled rate for 6 h.

Keywords: nanoparticles, glycerol, poly(methyl methacrylate), DEET, mosquito repellant

CMPS - 11

FABRICATION OF ELECTROCATALYST BASED ON PEDOT-PSS SUPPORTED Pd NANOPARTICLES FOR ETHANOL ELECTRO-OXIDATION

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\Studies related on the search for an effective yet less expensive catalyst and support material for fuel cells, constitute a step on the development of possible solutions to increase the efficiency of a Direct Ethanol Fuel Cell while lowering its cost. Palladium nanoparticles were synthesized via oleylamine-mediated synthesis and precursor method to achieve a mean particle size of 3.78 nm ± 0.45 nm and 3.63 nm ± 0.59 nm, respectively as revealed by transmission electron microscopy (TEM). Poly(3,4-ethylenedioxythiophene) doped with poly(styrene sulfonate) (PEDOT-PSS) was prepared by a simple chemical synthesis procedure and was used as a supporting matrix for the Pd nanoparticles (PdNPs). Two different methods to remove the capping agent during the synthesis of metal nanocatalysts were studied, i.e. acetic acid washing and thermal annealing. It was found out that both thermal annealing and acetic acid washing were effective in removing the capping agent, oleylamine. The study was successful in developing an electrode based on PEDOT-PSS supported Pd nanoparticles which gave a current density of 0.90 mA/cm^2 for ethanol oxidation in alkaline medium, which is relatively lower compared to the activity of PdNPs–CNTs (carbon nanotubes)/Naûon–GCE (glassy carbon electrode) reported in the literature. The prepared electrode showed electrochemical stability even up to 50 oxidation cycles. This study is an effort pointing towards the development and possible commercialization of non-platinum based fuel cell anode dispersed on a conductive polymer matrix.

Keywords: fuel cell, electrocatalyst, Pd nanoparticles, PEDOT-PSS, TEM

CMPS - 12

NANOWIRE FORMATION AND POLYMER CONFORMATIONS OF ELECTROPOLYMERIZED POLY(3,4-ETHYLENEDIOXYTHIOPHENE) (PEDOT) ON IODINE-MODIFIED Au(111) SINGLE CRYSTAL ELECTRODE AS PROBED BY *in-situ* STM

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In the field of nanotechnology, there is a growing interest in the synthesis of conjugated polymer nanowires because of their promising applications in nanodevices and molecular electronics. In this study, the electrochemical polymerization of 3,4-ethylenedioxythiophene (EDOT) ($E_{ox} = 1.20$ V) on iodine-modified Au(111) single crystal electrode in aqueous 0.10 M $HClO_4$ was investigated by cyclic voltammetry (CV) and electrochemical scanning tunneling microscopy (EC-STM). The Au(111) single crystal electrode was fabricated using the *Clavilier's* method. The iodine adlayer was prepared by dipping a freshly annealed Au(111) single crystal electrode in a 0.10 M potassium iodide (KI) solution.

Cyclic voltammetric and EC-STM data revealed the iodine adlayer was stable from E = 0.0 - 1.40 V vs. Reversible Hydrogen Electrode. This provided a suitable potential range for EDOT electropolymerization at 1.20 V vs. RHE. EC-STM was used to examine the formation of EDOT adlayer on iodine-modified Au(111) electrode. The iodine adatoms on Au(111) surface were prominent at negative potentials but EDOT molecules gradually appeared as bright spots when the potential was shifted more positively. However, the formation of an ordered adlayer of EDOT molecules was not observed. *In-situ* electropolymerization of EDOT was carried out at 1.20 V and showed the formation of single-molecular chains of PEDOT with diameter and lengths of 0.9 nm and 5-7 nm respectively. Extensive STM imaging further revealed PEDOT having bended polymer backbones of 105°, 144° and 180° (i.e hairpin folding). The growth of PEDOT multi-layers is observed when the potential was held for a longer time.

Keywords: Poly(3,4-ethylenedioxythiophene), nanowire, iodine, Au(111) single crystal electrode, scanning tunneling microscopy

CMPS - 13

MICROWAVE-ASSISTED REACTION: A CLEANER AND EFFICIENT METHOD FOR THE SYNTHESIS OF INDAZOLES AND BENZIMIDAZOLES

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The use of microwave radiation for heating reaction mixtures has proved to be a convenient method for the synthesis of indazoles and benzimidazoles as it can carry out the reaction under solvent-free condition, at shorter reaction time and with better product yield.

A domestic microwave oven was used to carry out the reactions. The starting materials were placed in a test tube and mounted in an Erlenmeyer flask. This set-up was placed inside the cavity of the oven and irradiated for several minutes at a particular power. The products were identified by their IR, ^{1}H nmr and ^{13}C nmr spectroscopic data.

A 77% yield of 2-phenyl-2*H*-indazole was obtained by irradiating a mixture of 1.0 mmol *N*-(2-nitrobenzylidene)aniline and 4.0 mmol $P(OEt)_3$ for 14 min at 200W. 2-(1-Naphthyl)-2*H*-indazole was obtained in 89% yield when *N*-(2-nitrobenzylidene)-1-naphthylamine and $P(OEt)_3$ was irradiated for 14 min at 200W. Irradiation of *N*-benzylidene-2-nitroaniline and PPh_3 for 5 min at 200W gave 96% 2-phenyl-1*H*-benzimidazole. Other indazoles and benzimidazoles were also synthesized using the microwave-assisted method. The results showed that high yields were obtained at shorter reaction times and without excessive use of organic solvents.

Keywords: microwave-assisted reaction, indazoles, benzimidazoles, imines, synthesis

CMPS - 14

METHOD VALIDATION FOR THE DETERMINATION OF IODINE IN URINE BY AMMONIUM PERSULFATE DIGESTION WITH SPECTROPHOTOMETRIC DETECTION OF THE SANDELL-KOLTHOFF REACTION

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Urinary iodine excretion (UIE) has been widely regarded as a biochemical marker for prevention and control of iodine deficiency disorders (IDD). To determine UIE levels, most methods require pretreatment of urine sample before its colorimetric detection based on the Sandell-Kolthoff reaction. In this study, a greener and safer oxidizing agent for the removal of iodide interferents in urine was used and validated. Three levels of pooled urine sample and a sample taken from the interlaboratory comparison used as control were analyzed for UIE using the ammonium persulfate method. Spectrophotometric detection of iodine in urine at 420 nm was performed after the addition of arsenous acid and ceric ammonium sulfate in the digested sample. The calibration curve was linear ranging from 0 – 800 μg/L. The detection limit was 0 μg/L and the quantitation limit was 0.2 μg/L urinary iodine. The method had an intra-assay coefficient of variation (CV) of 26.3% for the low, 4.1% for medium and 2.2% for high UIE level controls. The inter-assay CV resulting from inter-analyst and inter-instrument analyses were 15.7% and 3.8%, respectively. The validated method for urinary iodine determination is fast, safe and economical.

Keywords: urinary iodine, ammonium persulfate, Sandell-Kolthoff, validation, urine

CMPS - 15

DETERMINATION OF *Trans* FATTY ACID IN VIRGIN COCONUT OIL AND OTHER FATS AND OILS BY GAS CHROMATOGRAPHY

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Trans fatty acid (*t*FA) in fats and oils were identified to be a risk factor for CHD and was made mandatory requirement under the Nutrition Labeling (US NLEA, 2000 and Canada, 2003). The study aims to validate/ verify the AOCS Ch2a-94 Gas Chromatography (GC) method of *t*FA analysis for virgin coconut oil (VCO) and other fats and oil.

Precision and accuracy were determined using in-house food reference material (IFRM, Grape seed oil), 2 Food Analysis Proficiency Assessment Scheme Quality Control Test Material (FAPAS QCTM, Vegetable oil and Breakfast Cereal), and inter-laboratory test with foreign laboratory. Linearity, LOD and LOQ were determined by 5 level concentration using 10 different *tFA* standards. Twenty five VCO samples and 5 refined, bleached and deodorized (RBD) oils were studied.

The method was found to be precise and accurate with Horrat value of 1.8 which is within the acceptable criteria (<2) and %recovery of 78.03% (addition method) and 112% (QCTM). Inter-laboratory test showed 0.09% difference in IFRM analysis. The calibration curve was linear (0.9786 – 0.9992) at a concentration range of 0.0044 – 0.38 mg/mL. The LOD was 0.00255 mg/mL and the LOQ was 0.00851 mg/mL. Using the US NLEA guidelines, all VCO samples contained zero *tFA* while the RBD oils contained of up to 2.2g/100g oil *tFA*.

In conclusion, VCO contains zero *t*FA and the AOCS method can be used for *t*FA analysis in VCO and other fats and oils. The method can be recommended for *t*FA analysis of fats and oils from food products.

Keywords: *trans* Fatty acid, Virgin Coconut Oil, method validation, gas chromatography

CMPS - 16

METHOD VALIDATION OF PLASMA OR SERUM RETINOL ANALYSIS USING HIGH PERFORMANCE LIQUID CHROMATOGRAPHY UV/VIS DETECTION

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Validation of analytical methods is essential in the generation of data for biochemical assessment studies to obtain reliable results that can be satisfactorily interpreted. For this purpose, the validation of plasma or serum retinol using high performance liquid chromatography was performed according to the requirements of ISO 17025 by taking into consideration the different criteria such as linearity, instrument detection limit, limit of quantitation and detection, trueness, repeatability and reproducibility.

The validation was carried out by using 100 µL of plasma or serum with 100 µL of retinyl acetate in absolute methanol. It was mixed for 2 seconds and extracted twice with 500 µL of hexane. The combined extracts were dried up under the stream of nitrogen gas. It was redissolved in 100 µL of 4:1 methanol-dichloromethane and 50 µL aliquot was injected to HPLC-UV/Vis.

Results showed that elution time of retinol was at 3.090±0.014 minutes and calibration standards behaved linearly ($R^2 = 0.9994 \pm 0.0001$) over the calibration range of 0.37-6.66 mg of retinol. The accuracy of the method evaluated from the analysis of the certified reference material was 102.89%. The % RSD of repeatability and reproducibility of the method were 3.35 % and 3.76%, respectively. The detection limit was lower than the quantification limit and within the admitted performance range.

The results of the analysis performed to validate the analytical method for the determination of retinol in plasma or serum showed that they were within the performance criteria set for this method and they met the requirements of ISO 17025.

Keywords: plasma or serum retinol, high performance liquid chromatography, method validation

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ANALYSIS OF ECSTASY IN HUMAN URINE BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

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Ecstasy or n-methyl-3, 4-methylenedioxymethamphetamine (MDMA) is one of the most popular club drugs. This drug was invented to treat obesity but is currently placed under Schedule 1 of controlled substances. It is a psychoactive drug like methamphetamine or shabu.

Ecstasy in urine was analyzed using High Performance Liquid Chromatography (HPLC) with UV detection set at 254 nm. Chromatographic analysis was carried out with a Luna 5μ C18 reversed phase column and (87:5:5:3) water:methanol:acetonitrile:ammonium buffer as mobile phase at flow rate of 0.5 mL/min. Ephedrine was used as an internal standard. MDMA and ephedrine showed average retention times of ~2.5 min and ~2.8 min respectively. Analysis of 0.50 ppm MDMA had % coefficient of variation (% CV) of 0.57% for the retention time of MDMA and 6.6% for peak area. Inter-day analysis showed % CV of 2.2% for retention time and 3.68% for peak area. Linear response was obtained over the concentration range of 0.10 ppm–1.00 ppm. The limit of detection (LOD) was 0.03 ppm.

Different concentrations of MDMA were spiked in certified drug-free urine and a linear response at the same concentration range after liquid-liquid extraction with ether was also obtained. Gradient elution using (87:5:5:3) water:methanol:acetonitrile:ammonium buffer as mobile phase A and 100 % acetonitrile as mobile phase B was employed to improve separation of MDMA from ephedrine in urine matrix. Different spiked urine samples underwent the same extraction procedure with ether and recoveries ranged from 81–104%.

HPLC analysis of ecstasy could provide an alternative rapid method to detect this drug of abuse in human urine samples.

Keywords: n-methyl-3,4-methylenedioxymethamphetamine (MDMA), ecstasy, urine, HPLC, liquid-liquid extraction

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CHROMATOGRAPHIC ANALYSIS OF KETAMINE AND NORKETAMINE IN HUMAN PLASMA AND URINE SAMPLES

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In recent years, the illegal use of ketamine in the Philippines has risen and this drug is now included in the list of dangerous drugs under the Comprehensive Dangerous Drugs Act of 2002. Ketamine is a fast acting anesthetic that is mostly administered by veterinarians as an animal sedative. It is also used by anesthesiologists for pediatric and elderly patients as surgical anesthesia. Complications from the use of ketamine include hallucinations and confused states which contributed to the abuse of this drug.

Chromatographic analysis of ketamine and norketamine, its metabolite, was carried out using high performance liquid chromatography (HPLC) with UV detection at 210 nm on a C_{18} column. The mobile phase used was 30% acetonitrile and 70% phosphate buffer (0.03M, pH 7.2). Flow rate was 0.5 ml/min and oven temperature was set at 37 °C. The retention times of ketamine and norketamine were found to be at ~5.6 min and ~11.3 mins respectively. Reproducible results were obtained with CV (%) of 7.33 % or less. Linear response was obtained over a concentration range of 25 to 500 ppb. LOD for ketamine is 3.6 ppb while LOQ is 4.04 ppb. While for norketamine, LOD and LOQ values were 6.10 and 6.72 ppb respectively.

Ketamine and norketamine standards were spiked in blank urine samples or human plasma sample from volunteers with no ketamine use. Linear response was also obtained over the concentration range of 25 to 500 ppb. Liquid-liquid extraction was utilized for sample preparation. Average percent recovery of ketamine spiked in blank human urine was 85.0% while in spiked human plasma samples, it was 91.0%.

This HPLC method could be utilized for routine analysis of ketamine and norketamine in human urine or plasma samples.

Keywords: high performance liquid chromatography, ketamine, norketamine, human plasma, human urine

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HALOGEN-FREE, IMIDAZOLIUM BASED IONIC LIQUIDS FOR ORGANIC AND INORGANIC SYNTHESES

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Ionic liquids (IL) are designer solvents exhibiting negligible vapor pressure, high thermal stability, wide liquid range, and excellent ability to dissolve various inorganic and organic compounds.Typical ILs consist of N,N'- dialkylimidazolium cations and a wide variety of halide-based anions but the presence of halides in these ILs raise environmental concerns when the hydrolysis stability of the anion is poor or when a thermal treatment of the IL in use is necessary. In response to this, two series of halogen-free, 1-alkyl-3-methylimidazolium [RMIM] based ILs, [RMIM] Acetate and novel [RMIM] Lauryl Sulfate (LS), have both been prepared through a two step procedure: step (1) involves a reaction between 1-methylimidazole and the appropriate alkylbromide to yield [RMIM]Br and step (2) involves the exchange of the bromide ion in [RMIM]Br with sodium acetate or sodium LS to afford the halogen free ILs. A comparison of optical properties of 1-butyl-3-methylimidazolium [BMIM]LS and [BMIM]Br shows that the interesting excitation wavelength-dependent behavior observed in both ILs is typical of ILs bearing the imidazole moiety. The Diels-Alder reaction provides a means by which heterocyclic rings may be produced from acyclic precursors in a single step and the endoselectivity (endo:exo=91:1) and product yield (89%) obtained for the Diels-Alder reaction between cyclopentadiene and methyl acrylate in 1-hexyl-3-methylimidazolium [HMIM] Acetate is remarkably high. The control of the morphogenesis of gold nanoparticles leads to unique properties that are essential to applications such as catalysis and analytical sensing. [RMIM] LS has been utilized both as a solvent and as a stabilizing agent in the synthesis of anisotropic gold nanostructures and the morphogenesis of these gold nanostructures has been examined. Presence of [BMIM] LS stabilized the formation of Au nanoplates as well as intertwined Au nanoparticles and nanorods.

Keywords: ionic liquid, lauryl sulfate, Diels-Alder, stabilizing agent, morphogenesis

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ELEMENTAL AND ISOTOPIC CHARACTERIZATION OF JAPANESE AND PHILIPPINE POLISHED RICE SAMPLES USING INSTRUMENTAL NEUTRON ACTIVATION ANALYSIS AND ISOTOPE RATIO MASS SPECTROMETRY

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Rice is a staple food for most Asian countries such as the Philippines and Japan and as such its elemental and isotopic content are of interest to the consumers. Its elemental content may reflect the macronutrient reduction during milling or probable toxic elements uptake. Three Japanese and four Philippine polished rice samples in this study mostly came from rice bought from supermarkets. These rice samples were washed, dried and ground to fine powder. Instrumental neutron activation analysis (INAA), a very sensitive non-destructive multi-element analytical technique, was used for the elemental analysis of the samples and isotope-ratio mass spectrometry (IRMS) was used to obtain the isotopic signatures of the samples. Results show that compared with the unpolished rice standard NIES CRM10b, the polished Japanese and Philippine rice sampled show reduced concentrations of elements by as much as 1/3 to 1/10 of Mg, Mn, K and Na. Levels of Ca and Zn are not greatly affected. Arsenic is found in all the Japanese rice tested at an average concentration of 0.103 µg/g and three out of four of the Philippine rice at an average concentration of 0.070 µg/g. Arsenic contamination may have been introduced from the fertilizer used in rice fields. Higher levels of Br are seen in two of the Philippine rice at 14 and 34 µg/g with the most probable source being the pesticide methyl bromide. Isotopic ratio of ä^{13}C show signature of a C3 plant with possible narrow distinguishable signature of Japanese rice within -27.5 to -28.5 while Philippine rice within -29 to -30. More rice samples will be analyzed to gain better understanding of isotopic signatures to distinguish inter-varietal and/or geographical differences. Elemental composition of soil samples of rice samples sources will be determined for better understanding of uptake mechanisms.

Keywords: rice, INAA, IRMS, elemental, isotopic

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THE AVERAGE OF THE mth POWER OF L_m NORM OF ZERO-ONE POLYNOMIALS ON THE BOUNDARY OF THE UNIT DISC

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Let $n \geq 0$ be any integer and

$$\Phi_n = \left\{ p(z) = \sum_{i=0}^{n} a_i z^i : z = e^{i\theta},\ a_i = 0,1\ \forall\ 0 \leq i \leq n \right\}$$

$$\Psi_n = \left\{ p(z) = \sum_{i=0}^{n} a_i z^i : z = e^{i\theta},\ a_i = 0,1\ \forall\ 0 \leq i < n,\ a_n = 1 \right\}$$

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be the collection of zero-one polynomials over C of degree less than or equal to n and of degree exactly equal to n respectively. We denote $\|p\|_m$ to be the Lm norm of any polynomial $p(z)$ and $\rho_n(m)$ and $\omega_n(m)$ be the average of the mth power of Lm norms in Φ_n and Ψ_n respectively. It is known that the cardinality of Φ_n is 2^{n+1} and the cardinality of Ψ_n is 2^n hence $\rho_n(m)$ and $\omega_n(m)$ is given by

$$\rho_n(m) = \frac{1}{2^{n+1}} \sum_{p \in \Phi_n} \|p\|_m^m, \qquad \omega_n(m) = \frac{1}{2^n} \sum_{p \in \Psi_n} \|p\|_m^m$$

In this paper we derived the exact formula for and for various values of

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Keywords: Zero-One Polynomials, norm of polynomial

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SECURE DOMINATION IN A NETWORK: A PROTECTION STRATEGY

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The concept of secure total domination in graphs was investigated further. The study particularly considered a result obtained by Benecke et al. in a recent article. A counter example showed that such result is faulty. A rectification of this result was provided and some quick consequences of the same were stated. Secure total dominating sets in the join of graphs were also studied and some characterizations were generated.

The aforementioned new type of protection strategy in a given network was considered in this study. This strategy which uses a variant of domination in a network is more secure than the ones studied previously. Just like other existing strategies, the objective in this strategy is to evaluate or determine the minimum number of guards needed to protect a graph or network.

The following main results have been generated in this study:

1. Let X be a total dominating set in a connected graph G, $v \in X$, and $u \in V(G) \setminus X$. Then v X-defends u if and only if $epn(v;X)$ and $ipn(v;X)$ are contained in $N_G(u)$.
2. If $u \in epn(v;X)$ for some $v \in X$, then u is not X-defended.
3. Let X be a total dominating set in G. Then X is a secure total dominating set if and only if (i) $epn(v;X) = \varnothing$ for all $v \in X$, and (ii) for each $u \in V(G) \setminus X$, there exists $v \in X \setminus N(u)$ such that $ipn(v;X) \subseteq N(u)$.
4. Let G be a connected graph of order $n \geq 2$. Then $st(G) = 2$ if and only if there exist $x, y \in V(G)$ such that $xy \in E(G)$ and $N(x) = V(G) \setminus \{x\}$ and $N(y) = V(G) \setminus \{y\}$.
5. Let G and H be connected non-complete graphs of orders m and n, respectively. Then $\gamma_{st}(G+H) = 2$ if and only if at least one of the following holds: (i) $\gamma_{st}(G) = 2$ or (ii) $\gamma_{st}(H) = 2$, or (iii) $\Delta(G) = m - 1$ and $\Delta(H) = n - 1$.
6. Let G and H be connected non-complete graphs of orders m and n, respectively, and suppose $st(G+H) \neq 2$. Then $st(G+H) = 3$ if and only if at least one of the following holds: (i) $\gamma(G) = 2$, or (ii) $\gamma(H) = 2$, or (iii) $\Delta(G) = m - 1$ 1 or $\Delta(H) = n - 1$ (but not both).

Keywords: X-defended, secure, domination, total domination, join

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CONVEX DOMINATION IN THE COMPOSITION AND CARTESIAN PRODUCT OF GRAPHS

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The convex dominating sets in the composition and cartesian product of two connected graphs were characterized. It was shown that the convex domination number γ_{con} (G[H]) of a composition G[H] of two non-complete connected graphs G and H is equal to the clique domination number γ_{cl}(G) of G. The convex domination number

γ_{con} (G x H) of the cartesian product of two connected graphs was also studied. It was found out that this number is related to the convex domination numbers of the graphs involved.

Some results in an earlier work on convexity were used to characterize the convex dominating sets in the composition and cartesian product of two connected graphs. The concept of cyclic domination number was also defined as this was needed to obtain an expression for the convex domination number of a composition of graphs.

The following results were generated in this study:

1. Let G be a connected graph and K_n the complete graph of order n. A subset $C = \cup\{[\{x\} \times T_x]: x \in S\}$ of $V(G[K_n])$ is convex dominating in $G[K_n]$ if and only if the S is convex dominating in G.
2. Let G be a connected graph and K_n the complete graph of order $n \geq 1$. Then $\gamma_{con}(G[K_n]) = \gamma_{con}(G)$.
3. Let G and H be connected non-complete graphs with $\gamma_{cl}(G) \geq 2$. Then a subset $C = \cup\{[\{x\} \times T_x]: x \in S\}$ of V(G[H]) is convex dominating in G[H] if and only if the S is a clique dominating set in G and T_x is a clique in H for every $x \in S$.
4. Let G and H be connected non-complete graphs with $\gamma_{cl}(G) \geq 2$. Then $\gamma_{con}(G[H]) = \gamma_{cl}(G)$.
5. Let G and H be connected graphs of orders m and n, respectively. Then $\gamma_{con}(G \times H) = \min\{n\,\gamma_{con}(G),\ m\,\gamma_{con}(H)\}$.

Keywords: domination, convex, clique, composition, cartesian product

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VERTEX COVER OF SOME SUPERGRAPHS OF PLANAR GRID

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Let G be the cartesian product of paths $P_m = a_1a_2\ldots a_m$ and $P_n = b_1b_2\ldots b_n$. Vertex $(a_i, b\text{-}_j)$ of G is denoted by $c\text{-}_{ij}$. Let H be the supergraph of G formed by adding the edges $c_{uv}c_{st}$ if $|u - s| = |v - t| = 1$. Vertex set of H has a subset U such that all the edges of H are incident to some elements of U. Such subset is called a vertex cover of H. The vertex covering number of H, denoted by $\alpha(H)$, is the minimum cardinality of a vertex cover of H. Let q and r be the quotient and remainder, respectively, when n is divided by 2. If $n = 1$, then $\alpha(H) = \#m/2\#$. If $n > 1$ and $r = 0$, then $\alpha(H) = q\#3m/2\#$. If $n > 1$ and $r = 1$, then $\alpha(H) = q\#3m/2\# + \#m/2\#$.

Keywords: planar grid, cartesian product, supergraph, vertex cover, vertex covering number

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ON THE MAXIMUM OF GENERALIZED STIRLING NUMBERS OF THE FIRST KIND

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The generalized Stirling numbers of the first kind $F_{\alpha,\gamma}(n,k)$ were defined by means of the following limit relation

$$F_{\alpha,\gamma}(n,k)=\lim_{\beta\to 0}\frac{\left[\Delta_t^k(\beta t+\gamma\mid\alpha)_n\right]_{t=0}}{k!\,\beta^k}$$

where α,γ are real numbers and n,k are nonnegative integers. The limit, when evaluated completely, gives an explicit formula

$$F_{\alpha,\gamma}(n,k)=\sum_{0\le j_1<j_2<\ldots<j_{n-k}\le n-1}\prod_{q=1}^{n-k}\left(\gamma-j_q\alpha\right),$$

In this paper, we determine the index k in which the sequence $\left\{F_{\alpha,\gamma}(n,k)\right\}_{k=0}^{n}$ assumes its maximum value using the above explicit formula and the Erdos-Stone Theorem.

The following are the major results in this study:

(1) For real numbers and nonnegative integers n,k, the sequence is strictly log-concave, and, thus, unimodal.

(2) For real numbers and nonnegative integers n,k, the sequence is asymptotically normal.

(3) The maximum value of the sequence occurs at the index where

Keywords: Stirling numbers, strictly log-concave, unimodal, asymptotically normal, Erdos-Stone theorem

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ON *p,q*-DIFFERENCE OPERATOR

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The *p,q*-difference operator of degree *n*, denoted by $\Delta^n_{p,q,h}$, is a mapping that assigns to every function *f* the function defined by the rule

$$\Delta^n_{p,q,h} f(x) = \left[\prod_{j=0}^{n-1} (p^j E_h - q^j)\right] f(x), \quad n \geq 1.$$

When $p = 1$, this will give the known *q*-difference operator of degree *n*, and, when $q \to 1$ and $h = 1$, this will further give the usual difference operator of degree *n*. It is known that the usual difference operator satisfies the following formulas:

(i) $\Delta^n f(x) = \sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} f(x+k)$

(ii) Newton's Interpolation Formula $f(x) = \sum_{k=0}^{\infty} \frac{\Delta^k_h f(0)}{k!} (x)_k$

In this paper, we establish *p,q*-analogues of these two formulas using the *p,q*-difference operator of degree *n*, and apply them to obtain explicit formulas of the *p,q*-analogues of some Stirling-type numbers. These can also be useful in writing the generating functions of these *p,q*-analogues in a more compact form.

The following are the major results in this study:

(1) For all integers *n* e" 1, $\Delta^n_{p,q,h} f(x) = \sum_{k=0}^{n} (-1)^k p^{\binom{n-k}{2}} q^{\binom{k}{2}} \begin{bmatrix} n \\ k \end{bmatrix}_{pq} f(x+(n-k)h)$

where $\begin{bmatrix} n \\ k \end{bmatrix}_{pq} = \prod_{i=1}^{k} \frac{p^{n-i+1} - q^{n-i+1}}{p^i - q^i}$ is called the *p,q*-binomial coefficient.

(2) A *p,q*-analogue of Newton's interpolation formula is given by

$$f_{q/p}(x) = a_0 + a_1 p^{x_0+1} \frac{[x - x_0]_{pq}}{p^x} + a_2 p^{2x_0-h+2} \frac{[x - x_0]_{pq}[x - x_1]_{pq}}{p^{2x}} + \cdots + a_m p^{mx_0-\binom{m}{2}h+m} \frac{[x - x_0]_{pq}[x - x_1]_{pq} \cdots [x - x_{m-1}]_{pq}}{p^{mx}}$$

where $$a_k = \frac{p^{k(k-1)} \Delta^k_{p^k,q^k,h} f_{q/p}(x_0)}{[kh]_{pq}[(k-1)h]_{pq} \cdots [h]_{pq}}$$

Keywords: *p,q*-difference operator, Stirling-type numbers, generating functions, Newton's interpolation formula, *p,q*-binomial coefficient

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SOME CHARACTERIZATIONS OF THE DIRECT PRODUCT OF GASSMANN TRIPLES

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In a finite group G, two subgroups H_1 and H_2 are Gassmann equivalent if each conjugacy class of G intersects H_1 and H_2 in the same number of elements. The triple (G, H_1, H_2) is then called a Gassman triple. This definition is equivalent to the well-known Sheng Chen's criterion for Gassmann equivalence. This paper considers this said criterion and a result on transitivity of Gassmann triples as tools in investigating some of the properties a Gassmann triple may satisfy with respect to direct product of Gassmann equivalent subgroups.

If (G, H_1, H_2) is a Gassmann triple, then Sheng Chen's Criterion guarantees the existence of a bijective function $\varphi: H_1 \rightarrow H_2$ such that $\varphi(h)$ is in the conjugacy class of h for all elements h of H_1. It also shows that (G, H_2, H_1) is a Gassmann triple. With an example of a Gassmann triple in hand, one asks whether the group in consideration contains another Gassmann triple and that the transition of these triples also form a Gassmann triple.

Results of this paper

1. If (G, H, K) and (G, H, L) are Gassmann triples, then (G, K, L) is also a Gassman triple.
2. If (G, H, K) is a Gassmann triple, then (GxG, HxH, KxK) is a Gassmann triple.
3. If (G, H, K) and (G, H, L) are Gassmann triples, then (G, HxK, HxL) is a Gassmann triple.
4. If (G, H, K) and (G, H, L) are Gassman triples, then (GxG, HxH, KxL) is a Gassman triple.

The last result is extended into a finite number of factors as follows:

5. Let (G, H, K_1), (G, H, K_2), … , (G, H, K_n) be Gassmann triples. Then ($\prod$G, H, $\prod K_i$) is a Gassmann triple.

Keywords: conjugate subgroups, conjugacy class, sheng chen's criterion, gassmann triple, gassmann equivalent subgroups, direct product of subgroups

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THE MINIMAL CLOSED GEODETIC NUMBERS OF GRAPHS

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Given two vertices u and v of a connected graph G, the closed interval $I_G[u, v]$ is the set of all vertices lying in some u-v geodesic in G. If S †" $V(G)$, then $I_G[S]$ = *" { $I_G[u, v] : u, v$ " S } . A set S of vertices in G is called a geodetic cover of G if $I_G[S] = V(G)$. The geodetic number $gn(G)$ of G is the minimum cardinality of a geodetic cover of G. A geodetic cover of smallest cardinality is called a geodetic basis of G. Suppose that in constructing a geodetic cover of G, we select a vertex v_1 and let $S_1 = \{ v_1 \}$. Select a vertex v_2 '"v_1 and let $S_2 = \{ v_1, v_2 \}$. Then successively select vertex v_i " $I_G[S_{i-1}]$ and let $S_i = \{ v_1, v_2, \ldots, v_i \}$. The closed geodetic number $cgn(G)$ and the upper closed geodetic number $ucgn(G)$ of G is the smallest and the largest k, respectively, for which selection of v_k in the given manner makes $I_G[S_k] = V(G)$. A closed geodetic cover S of G is a minimal closed geodetic cover of G if no proper subset of S is a closed geodetic cover of G. The minimal closed geodetic number $mcgn(G)$ is the maximum cardinality of a minimal closed geodetic cover of G. In this paper, it is shown that $ucgn(G) = mcgn(G)$ if and only if G is complete, while $cgn(G)$ and $mcgn(G)$ coincide among extreme geodesic graphs G. Moreover, for complete bipartite graphs $K_{m,n}$, $cgn(K_{m,n}) = mcgn(K_{m,n})$ if and only if $m = n$. More interestingly, for every triple a, b, c " Z^+, with 2 d" $a < b < c$, a, b, and c are realizable as closed geodetic number, minimal closed geodetic number, and upper closed geodetic number, respectively, of a connected graph. We also determined here the minimal closed geodetic numbers of graphs resulting from the join of graphs.

Keywords: geodetic number, bipartite graph, geodetic cover

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THE QUANTUM PROPAGATOR OF THE HARMONIC OSCILLATOR WITH DAMPING: A WHITE NOISE PATH INTEGRAL APPROACH

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Recently, the infinite dimensional white noise calculus by T. Hida and L. Streit has successfully provided a more mathematically well-defined formulation to the Feynman path integral. It has already been successful in solving quantum problems such as the perturbed harmonic oscillator and systems with exponentially-growing potentials. In this paper, white noise analysis is utilized to solve the quantum propagator, expressed as the Feynman path integral, for the harmonic oscillator with damping described by the Caldirola-Kanai Lagrangian, $L = \frac{1}{2} m\exp(\gamma t)\dot{x}^2 - \frac{1}{2} m\exp(\gamma t)\nu^2 x^2$ for a particle of mass m and angular frequency, ν, which is subjected to a damping of constant γ. In this approach, a parametrization of the paths of the particle in terms of an exponentially decreasing Brownian motion was employed thereby reformulating the Feynman path integral in the context of white noise analysis where the *S*- and *T*- transforms in white noise calculus are then used to evaluate the integral. The calculated propagator agrees with known results. The time-dependent wave function for the harmonic oscillator with damping is then extracted via the symmetrization of the calculated propagator which also agrees with known results.

Keywords: white noise analysis, propagator, harmonic oscillator with damping, Caldirola-Kanai Lagrangian, path integral

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SURFACE MODIFIED ZINC OXIDE: A POTENTIAL SMOKE SENSOR AT AMBIENT CONDITION

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Zinc oxide (*ZnO*), with its satisfactory stability, has been extensively used as a gas sensor for various gases such as hydrocarbons, oxygen, H_2O, *etc*. *ZnO*-based gas sensors are usually operated at >100°C temperatures which demand more power consumption compared to sensors that can operate at room temperature. To our knowledge, no reports have been presented on the capability of surface modified bulk *ZnO* to sense smoke at ambient condition. In this study, the smoke sensing properties of *HCl*-etched *ZnO* samples in pellet form is presented.

ZnO powders (99%) were pelletized and annealed at 700-1000°C with 100°C increment. Acidic etching using appropriate amount of hydrochloric acid was performed to increase the surface area of the samples. Morphology, electrical and smoke sensing characteristics of the surface modified *ZnO* pellets were investigated at room temperature (~25°C). Electrical stability of the annealed samples improves as the annealing temperature is increased. All samples have n-type conductivity which is intrinsic for *ZnO*. Increase in surface area through etching was successfully achieved as seen from their scanning electron microscope (SEM) images. These *HCl*- etched *ZnO* pellet samples are then referred to as surface modified samples. The surface modified *ZnO* pellets are more sensitive to smoke than the as-annealed *ZnO* pellets. The remarkable increase of sensitivity from ~11 to ~2000% is exhibited by the surface modified *ZnO* pellets annealed at 700°C. These results indicate that *ZnO* is a potential material for smoke sensing application at ambient condition.

Keywords: zinc oxide, smoke sensor, annealing, etching, sensitivity

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THE EFFECT OF ADHESION FORCE ON CELL ELASTIC MODULUS

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The ability of cells to deform or resist deformation affects several important factors of cell function. Most studies infer the elastic modulus of a living cell from the simultaneous measurements of forces and deformations exerted on the cell, based on the Hertz model. However, the force-distance curves are affected by indenter-cell adhesion forces, and neglecting this effect may result in systematic errors in the determination of the Young's modulus of elasticity.

For the first time, the Hertz model was extended to include the effect of adhesion in the description of contact stiffness by using the Lennard-Jones potential to model the inter-molecular interaction between the probe surface and a living cell sample. The adhesion force derived from the potential gradient was incorporated to the Hertz relation, from which the value of the elastic modulus of the sample is obtained.

Our results show that during indentation of the intact cell, the adhesion force increases in proportion to the indentation depth. The increase in the slope of the force-indentation curves predicts a higher Young's modulus than the value obtained by the Hertz model neglecting adhesion force by up to 25% for decreasing size of molecules coating the probe. The model predicts the Young's modulus of a cell based on the radius of the probe, and the size and concentration of the molecules coating the surface. Thus, our approach provides precision on cell mechanics measurements without neglecting surface interactions that could be incorrectly neglected.

Keywords: Young's modulus, Hertz model, Lennard-Jones potential, elastic force, force-indentation curve

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HIGH RESOLUTION PROBING OF ELASTIC PROPERTIES OF BIOPOLYMERS AND LIVING CELLS

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Correlation measures based on embedded probe fluctuations, are now widely used for characterizing viscoelastic properties of biological samples. However, novel applications using this robust tool are still lacking, considering that the study of living matter routinely demonstrate new phenomena, not immediately characterized by usual quantitative tools. Therefore, we derived new experimental and theoretical approaches to adapt ways of probing non-linear and non-equilibrium phenomena for biological samples.

Optical tweezer systems, two-beam tandems using dual-wavelength and single-wavelength splitting, were designed for high resolution microrheology in bulk down to single biopolymer or protein, based on the fluctuation spectra of embedded or attached probes. We derived calculations for winding turn probabilities to account for unfolding events in single fibrous biopolymers and globular proteins under tensile stretching based on approximating the ensuing probe fluctuations as originating from a damped harmonic oscillator under oscillatory forcing. Furthermore, for networks of biopolymers and living cells, we designed experiments using force pulses for simulating non-equilibrium phenomena, which naturally incorporates non-linear mechanics. The tools developed in this study will probe elastic properties of single biopolymers and networks, as well as living cells, aimed to gain insights for creating low-cost technologies for industrial and medical applications.

Keywords: biophysics, microrheology, biopolymers, cell mechanics, biomechanics, protein folding, non-equilibrium phenomena

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ELASTIC PROPERTIES OF A BIOPOLYMER

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The mechanical and dynamical properties of a cell are primarily determined by the network of biopolymers in the cytoplasm and the nucleus. Furthermore, these constituent biopolymers play an important role in biological functions, such as in facilitating molecular transport within the intracellular environment, in changing structure for movement, and in providing mechanical support to maintain shape. The cell's physiological behaviour, which collectively contributes to the organism's health, is therefore linked with the interplay of intracellular biopolymers. Since each biopolymer in a cell contributes to cell mechanical properties, understanding the physics behind the adaptive elasticity of individual biopolymers is crucial in gaining biological insights on emergent cellular behaviour.

In this study, the elastic properties of a single biopolymer under tensile stress were investigated, deriving an elasticity model that is valid beyond thermal regimes.

This novel elastic model was shown to predict the behaviour of stretched double-stranded deoxyribonucleic acid, single-stranded deoxyribonucleic acid, single-stranded ribonucleic acid, and titin in recent experiments. The model uses the persistence length, which is proportional to the bending rigidity, considering thermal fluctuations, and is validated at minimum bending mode of truncated polynomial expansion. Our newly derived elasticity model fits a broader range of force-extension relations in various types of biopolymers, compared to existing wormlike chain and freely jointed chain models. Therefore, our approach is generically applicable to biopolymers and is applicable to industrial polymers of similar properties.

Keywords: elasticity, biopolymers, cell mechanics, persistence length, bending rigidity, wormlike chain, freely jointed chain, double-stranded, single-stranded, titin, bending mode

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EFFECTS OF APPLIED VOLTAGE ON THE MEAN DIAMETER OF ELECTROSPUN POLYANILINE (PANI)-ELASTOMERIC ADHESIVE FIBERS

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The effects of applied voltage on the mean diameter of electrospun polyaniline (PANI)-elastomeric adhesive fibers were investigated. Polymeric solutions composed of equal volume of dimethyl sulphoxide-dissolved polyaniline and elastomeric adhesive were prepared. These solutions were drawn into fibers by electrospinning with different applied voltages of 20, 30, 40, 50, and 60 kV. Scanning Electron Microscopy (SEM) images, together with fiber diameter measurements, showed that as the applied voltage was increased, the mean fiber diameter of the electrospun fibers also increased. The increase in mean fiber diameter was attributed to shortened flight time of the jets produced during electrospinning, increased deposition rate and bead formation, which contributed to the increase in fiber diameters.

Keywords: conducting polymer, elastomeric adhesive, electrospinning, polyaniline

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WHITE NOISE PATH INTEGRAL APPROACH ON THE PARTITION FUNCTION OF A SEMI-FLEXIBLE BIOPOLYMER IN A BEND AND TWIST WORM-LIKE CHAIN MODEL

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Understanding the elastic behavior of biopolymers is helpful in understanding biological processes like gene regulation and transcription in cells. Thus, in recent years, statistical mechanics of biopolymers has emerged as a field of rapid theoretical and experimental investigation. This interest has been motivated from experiments which probe the function of elasticity of these biopolymers.

In this paper, we investigate the partition function of a semi-flexible biopolymer theoretically modeled in a Worm-Like Chain (WLC) model which considers its bend and twist degrees of freedom. We note that this partition function can be expressed as $Z=\exp(\beta f)Z_{x1}Z_{x2}$, where $\beta=L/s_b$ is the ratio of the biopolymer's contour length L to its bend persistence length s_b, $f = s_bF/k_BT$ is the applied force F in units of k_BT/s_b, and Z_{x1} & Z_{x2} are path integrals of the form

$$Z_{x_n} = \int D[x_n] \exp\left(i \int_0^{\beta'} \left[\frac{1}{2}\dot{x}_n^2 - \frac{(f-\tau^2/4)}{2} x_n^2 \right] d\zeta \right) \qquad (1)$$

where $\beta' = i\beta$ and τ is the torque applied to the system. We note that Eq. (1) is similar in form to the quantum mechanical propagator of a harmonic oscillator and we then solve this expression of Z_{xn} using the White Noise Path Integral Approach (WNPIA) pioneered by T. Hida and L. Streit. After which, a final form of the partition function is obtained. Following the works of A. Ghosh, we then derived the mean-extension of the biopolymer from this final form of partition function and plotted it as a function of applied force and torque. As expected, it was found out that for a fixed value of the torque the mean-extension increases as the pulling force is increased whereas it decreases when the torque is increased while the pulling force is kept fixed. Also, it was noted that even at a zero force, there was a nonzero mean-extension of the biopolymer. The results in this paper basically agreed with the works of A. Ghosh.

Keywords: partition function, semi-flexible biopolymer, bend and twist WLC model, WNPIA, mean-extension, quantum mechanical propagator

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STRETCHING SINGLE MOLECULAR DNA BY TEMPERATURE GRADIENT: A WHITE NOISE FUNCTIONAL APPROACH

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In this study, we obtained the mechanical properties of double stranded DNA (dsDNA) particularly the partition function and extension under small fluctuations limit stretched by temperature gradient field with Wormlike Chain (WLC) as the favored theoretical model. In this model, the dsDNA is treated as a continuous curve chain. The Hida-Streit integral formulation (White Noise Analysis) is used as a tool in evaluating the partition function of the dsDNA under temperature gradient field because of its versatility and prowess in solving many problems in quantum mechanics as well as in statistical mechanics which includes the system focused in this study. From the partition function, the extension or dsDNA's elastic response through stretching is calculated which turns out to be linearly dependent on the temperature gradient field strength. The result of the calculation shows that temperature gradient can exert force on dsDNA and create internal tension within it which is enough to study and manipulate the biomolecule.

Keywords: partition function, dsDNA, wormlike chain model, temperature gradient, white noise analysis

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INITIAL STUDIES OF A MICROWAVE-INDUCED ATMOSPHERIC PLASMA JET

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This study investigates the dimensions of plasma using a 6kW microwave-induced atmospheric plasma jet. The forward power studied ranges from 600W to 1800W for different flow rates. In this experiment, a 9.5cm quartz glass was used. In order to measure the length of the plasma, images of the plasma for different settings were observed using a digital camera 127cm away from the setup. The data is presented as plasma length versus absorbed power. It was shown that the plasma length increased as the absorbed power was increased. It was also observed that the ambient air had an influence on the plasma length. The results of this study are relevant for future optimization studies involving the microwave plasma jet.

Keywords: atmospheric plasma, microwave, plasma jet, plasma length, optimization

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INFLUENCE OF STACKED Ge ISLANDS ON THE DARK CURRENT-VOLTAGE CHARACTERISTICS OF A DIODE FOR SOLAR CELL APPLICATION

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We report on the dark current-voltage (*I-V*) characteristics of the diode with embedded stacked Ge islands in the intrinsic layer for solar cell application. Gas-source molecular beam epitaxy was used to grow the stacked Ge islands on a Si substrate. Two-diode model was utilized to analyze the dark *I-V* characteristics of a solar cell with embedded Ge islands in the intrinsic region. This model describes the relationship between current and voltage of a solar cell with stacked Ge islands in the generation region under dark condition. Furthermore, this model is capable of predicting some physically meaningful parameters for the enhancement of solar cell efficiency. Based on this two-diode model, we found out that the minority carrier diffusion and the recombination current components increase when there is an increase on the number of stacked Ge island layers. Moreover, we believe that the increase in minority carrier diffusion current might be due to an increase on the intrinsic carrier density as the number of stacked Ge island layers increases. Similarly, the increase in the recombination current components might be due to the enormous recombination of carriers in the intrinsic region as the number of stacked layer increases. These results can be used to fabricate a high-efficiency solar cell with embedded stacked Ge islands through efficient separation of electron-hole pairs by the internal electric field and this can contribute to significantly increase the photocurrent without considerable recombination of carriers in the stacked Ge island layers.

Keywords: p-n junction; two-diode model; Ge islands; solar cells

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ANISOTROPIC SURFACE TEXTURING OF SILICON SUBSTRATE USING ALKALINE SOLUTION FOR SOLAR CELL APPLICATION

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High-efficiency silicon solar cells need a textured front surface to reduce the reflectance of incident light and to improve light trapping using cost-effective method. In this work, we report on the anisotropic surface texturing of Si(100) substrates using alkaline solution, forming pyramidal structures on its front surface. This method provides a straight forward and cost-effective approach. We utilized a mirror-polished single crystalline Si(100) substrate for texturing using alkaline solution. The alkaline mixtures contained sodium hydroxide, isopropyl alcohol and de-ionized water. The concentration of the alkaline solution was held constant while varying the texturing time. The surface morphology of the textured surface is investigated by Scanning Electron Microscopy (SEM) and its reflectance is measured using UV-Vis Spectrometer. Results showed that the sizes and shapes of the resulting pyramids after texturing process are dependent on the texturing time. Furthermore, the pyramid density increases with increasing etching time. Moreover, SEM images revealed that the size and the uniformity of the pyramids affect the reflectance of the incident light as depicted in the UV-Vis spectra of the mirror-polished and textured silicon samples. It was found that reflectance of the incident light could be reduced up to less than 20 percent by optimizing the surface morphology of the textured silicon. It is suggested that having a large and almost uniformly distributed pyramids on the Si surface will drastically reduce the reflectivity. We also present in this study a model that will describe and discuss the effects on the reflectance in relation to the distribution of pyramids in terms of distance and size.

Keywords: solar cells; anisotropic surface texturing; reflectivity; alkaline solution

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PERFORMANCE EVALUATION OF TAILOR MADE MICROSPHERES AS SENSING LAYER RESPONSIVE TO RESIDUAL CHLORAMPHENICOL IN FOOD MATRICES

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Antibiotics like chloramphenicol are banned in food products of animal origin. Analysis of trace levels of chloramphenicol usually by GC-MS is expensive and could require tedious samples preparation. In this work, chloramphenicol-imprinted microspheres were synthesized via precipitation polymerization at 60°C using chlorampenicol as the template, and methacrlic acid as the monomer. Different crosslinkers like trimethylolpropane trimethacrylate (TRIM), ethylene glycol dimethacrylate and divinylbenzene were tried to produce the polymer. Their binding characteristics were evaluated by Scatchard analysis using UV VIS spectrophotometer. Two classes of binding sites were obtained under the concentration studied. From these polymer microspheres bearing the imprinted sites, the one prepared with TRIM crosslinker showed the highest binding capacity than the non-imprinted polymer and polymers prepared using other crosslinkers. The maximum binding sites were estimated to be about 330 μg/g and 268 μg/g for the molecularly imprinted polymer and the non-imprinted polymer respectively. The adsorption isotherm of the imprinted polymer was fitted to the Freundlich equation and the heterogeniety index was estimated to be about 0.976. Molecular capability of the said polymer as sensing layer to trace amount of chloramphenicol was also confirmed by gravimetric technique using a mass sensor. Results of sensor measurement obtained shows good accuracy and acceptable percent recovery in real samples. Further characterization of the resulting polymers were also performed using BET surface area analyzer, particle size analysis, and microscopic techniques. The study gives merit to the quality of spherical particulates in nano to micro size range. The proposed integration of this polymerization technique and sensor technology can be carried out for very minute analysis of chloramphenicol much quickly with simple sample preparation. **These polymers can also be utilized in sample screening and as effective adsorbent in separation processes.**

Keywords: chloramphenicol, Scatchard analysis, molecularly imprinted microspheres, precipitation polymerization, chemical mass sensor

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A MONTE CARLO SIMULATION STUDY ON THE INTERACTIONS OF PROTON, ^{7}Li AND ^{12}C WITH WATER FOR HADRON THERAPY APPLICATION

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The interactions of ^{12}C, ^{7}Li and protons were simulated using a tissue reference media (water). The primary focus is to investigate the nuclear fragmentation which is believed to be the cause of the so-called dose-tail located right after the Bragg peak structure, which might affect the healthy neighboring tissue of the tumor.

Using Monte Carlo Method in GEANT4 (GEometry ANd Tracking 4th incarnation) toolkit, a pencil-like beam profile with Gaussian energy distribution is directed towards a box-shaped water target. Mean energies ranging from 100 MeV to 400 MeV for ^{12}C, 100 MeV to 250 MeV for the ^{7}Li, and 50 to 250 MeV for protons were used. Electromagnetic (EM) interactions are described by the standard and low-energy EM models, while the nuclear fragmentation interactions are described by the Hadronic interaction models such as the Binary cascade and Statistical Multifragmentation Models. Information such as Depth dose profile and peak to entrance ratio were extracted from the simulation.

The results show that the peak-to-entrance ratio was lower at higher mean energies for the three projectiles. At 400 MeV the peak-to-entrance ratio was about 3.425 for ^{12}C. At 250 MeV the peak-to-entrance ratio were 3.615 and 2.514 for protons and ^{7}Li, respectively. These peak-to-entrance values are approximately half of the highest known value of ^{12}C at 175 MeV. Unlike protons, ^{12}C and ^{7}Li produced a larger dose tail with ^{7}Li lower by 37.88% than ^{12}C at 170 mm range.

Results suggest that for the three projectiles it is ^{7}Li which are most suitable for therapeutic radiation therapy since it has lower dose tail compared to ^{12}C and a more enhanced peak-to-entrance ratio compared to proton.

Keywords: hadron radiation therapy, nuclear fragmentation, dose tail, peak-to-entrance ratio, Bragg peak

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ANGULAR AND LATERAL RESOLUTION STUDY IN pCT IMAGING INVOLVING BIOLOGICAL TISSUES

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The angular and lateral resolutions were studied for possible application in proton Computed Tomography (pCT) imaging which is a prerequisite procedure for radiation therapy. These quantities provide a measure of the sharpness of the image using proton beams but unlike the conventional x-ray imaging, protons suffer from deflections due to multiple Coulomb scattering (MCS) interactions. In order to improve pCT images, analytical formulas that model the effect of MCS on individual proton trajectories were investigated.

The standard deviation of the angular (σ_u) and lateral (σ_y) distributions were calculated using analytical MCS models reported in two journals: (a) *Phys. Med. Biol., 49 (2004), 2899-911* and (b) *Med. Phys., 35 (2008), 4849-56*. In this study, two methods were performed: the numerical method and the sampling method.

During the simulation, a pencil beam profile of protons is directed to a cubic phantom (20 cm^3 for water, soft tissue or muscle tissue and 10 cm^3 for compact bone) using the Geant4 toolkit. Fifty thousand protons were bombarded at incident energies 200 MeV and 250 MeV. A 5th order polynomial was then used to parameterize the energy loss function. To test the validity of the analytical models, the angular and lateral distributions were obtained by Monte Carlo sampling of the exit protons. The σ_u and σ_y were extracted and compared with the result of the analytical method.

Results show that for a 200 MeV incident proton, the angular and lateral scattering was around 2 degrees and 3.27 mm, respectively, while for the 250 MeV the values were 1.38 degrees and 2.5 mm, respectively. Also, the inclusion of a logarithmic correction factor to the MCS model improved the analytical σ_u and σ_y values with an error of about 17%. In conclusion, good resolution was observed at higher energies.

Keywords: proton computed tomography, pct, mcs, lateral resolution, angular resolution