CHEMICAL MATHEMATICAL AND PHYSICAL SCIENCES DIVISION

CMPSD No. 1
SUBDIVISION NUMBERS OF THE CLOSURE OF SOME GRAPHS

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The *closure* $c(G)$ of a graph G of order p is the graph obtained from G by recursively joining pairs of non-adjacent vertices whose degree sum is at least p until no such pairs remain. 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 $|x-y|=1$, satisfy, where $|x-y|$ denotes the Euclidean distance between x and y.

The *subdivision number* of a graph G, denoted by $sd(G)$, is the minimum number of vertices to be inserted into the edges of G to make it isomorphic to a unit graph in In 1998, Gervacio and Maehara found the subdivision numbers of the complete graph and the complete bipartite graph. The subdivision numbers of the closure of some graphs are determined in this study.

For the closure of the cycle, the wheel, and the fan, we obtain the following results:

i) $$sd(c(C_n)) = \begin{cases} 0 & \text{if } n \neq 4, \\ 2 & \text{if } n = 4. \end{cases}$$

ii) $$sd(c(W_n)) = sd(c(F_n)) = \begin{cases} 2 & \text{if } n = 3, \\ 4 & \text{if } n = 4, \\ 8 & \text{if } n = 5, \\ 0 & \text{if } n = 6. \end{cases}$$

iii) $$\text{for } n \geq 7,\ sd(c(W_n)) = \left\lceil \frac{n}{6} \right\rceil \text{ and } sd(c(F_n)) = \left\lfloor \frac{n-1}{6} \right\rfloor$$

Keywords: closure, unit graph, subdivision number

A BER EXPRESSION FOR A CHANNEL WITH AWGN AND ACI

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Abstract

We present a closed form expression for the average bit error rate (BER) for a binary phase-shift keying (BPSK) modulated signal corrupted with additive white Gaussian noise (AWGN) with adjacent channel interferrence. The simplest mathematical model for a communication system is the additive white Gaussian noise channel, where the transmitted signal is corrupted by additive random process $n(t)$, resulting in a received signal in the form $r(t) = s(t) + n(t)$, where $n(t)$ is a random process with zero mean and variance $N_0/2$. If ACI is added into the model, the received signal is $r(t) = s(t) + n(t) + a(t)$, where $a(t)$ is ACI component. We consider two cases: we first assume that noise from the adjacent channel is constant, i.e., $a(t) = \alpha$, and also consider the case when $a(t)$ is a random process. To create a closed form BER for the two cases, we take the convolution of the distributions of $n(t)$ and $a(t)$, and we identify the conditional pdfs corresponding to each BPSK signal. For the constant case, the average BER was found to be

$$\bar{\varepsilon} = Q(2\rho)\,,$$

which is the theoretical BER for AWGN with no ACI (here, Q is Q-function). For the case where $a(t)$ is a random process, we assume a trigonometric probability distribution given by

$$f_a(z) = \begin{cases} \dfrac{1}{\pi\sqrt{\alpha^2 - z^2}}\,, & |z| < \alpha\,, \\ 0\,, |z| \geq \alpha\,, \end{cases}$$

where we let z be the random ACI variable with magnitude α. The BER

obtained for this case is

$$\bar{\varepsilon} = \frac{1}{2\sqrt{\pi^3 N_0}}\left[\int_{-\infty}^{0}\int_{-\alpha}^{\alpha}\frac{e^{\frac{-(z-\sqrt{E_b}-z\xi)^2}{N_0}}}{\sqrt{\alpha^2-\xi^2}}dzd\xi + \int_{0}^{\infty}\int_{-\alpha}^{\alpha}\frac{e^{\frac{-(z+\sqrt{E_b}-z\xi)^2}{N_0}}}{\sqrt{\alpha^2-\xi^2}}dzd\xi\right],$$

where ξ is the random Gaussian variable and E_b is the BPSK signal energy.

Keywords: BPSK, BER, AWGN, convolution

CMPSD No. 3

CHARACTERIZATION OF SEMI-CONTINUITY IN THE CARTESIAN PRODUCT

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N. Levine introduced the concepts such as semi-open set and semi-continuity in topological spaces. The class of all semi-open sets in a topological space includes all open sets. Although an arbitrary unions of semi-open sets is semi-open, the class does not always form a topology on the underlying set.

Now, given a family of topological spaces $\{Y_\alpha : \alpha \in \Omega\}$ and a function f from a topological space X into the Cartesian product Y of the spaces Y_α with the Tychonoff topology, it is well known that f is continuous if and only if each coordinate function $p_\alpha \circ f$ is continuous. In this paper, we give a necessary and sufficient condition for function f to be semi-continuous. More precisely, the results obtained are as follows:

(1) If O is a non-empty semi-open set in the Cartesian product space Y, then $p_\alpha(O) = Y_\alpha$ for all but at most finitely many α and $p_\alpha(O)$ is semi-open for every $\alpha \in \Omega$.
(2) Let $S = \{\alpha_1, \alpha_2, ..., \alpha_t\}$ be a finite subset of Ω and $O_{\alpha_i} \subseteq Y_{\alpha_i}$ for each $\alpha_i \in S$. Then $< O_{\alpha_1}, O_{\alpha_2}, ..., O_{\alpha_t} >$ is semi-open in Y if and only if each is O_{α_i} semi-open in.
(3) Let X be an arbitrary space and Y the product space. A function $f : X \to Y$ is semi-continuous on X if and only if each coordinate function $p_\alpha \circ f$ is semi-

continuous on X.

(4) Let X and Y be product spaces of the families $\{X_\alpha : \alpha \in \Omega\}$ and, $\{Y_\alpha : \alpha \in \Omega\}$ respectively. For each $\alpha \in \Omega$, let $f_\alpha : X_\alpha \to Y_\alpha$ be a function. If each f_α is semi-continuous on X_α, then the function $f : X \to Y$ defined by is semi-continuous on X.

Keywords: topology, subbase, base, open set, semi-open set, continuous, semi-continuous, Tychonoff topology, product space

CMPSD No. 4

NUMERICAL COMPUTATIONS FOR PARAMETER ESTIMATION IN A SMART BEAM STRUCTURE

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We present a method to estimate the parameters of a smart beam structure. The data consists of beam displacements taken at di_erent time instances but due to unavailability of an actual experimental setup, we will use numerically simulated data. The model used is the Euler-Bernoulli equation modified to include internal damping and passive actuator contributions. Piezoceramic patches were used as the smart materials. The parameters we estimate are the density, stiffness and damping of both the beam and patches, and also the dielectric constant of the patches. The first step is to numerically discretize the PDE describing the vibrations of the beam. The Galerkin approximation method using cubic splines as basis functions is used. Then, numerically simulated data is collected by simulating the PDE and recording numerical displacements at one point on the beam and at different time instances. The parameters used in simulating data will be the \true" parameters of the system. Then we formulate the cost function that returns the difference between data and numerical displacements. Finally, the Nelder-Mead optimization algorithm is used to obtain the minimizer of the cost function. Numerical results show that the method can obtain the \true" or \estimated" parameters of the system even if noise is added onto the data. We were also able to determine that the initial guess supplied to the numerical optimizer can have an error (i.e., difference from the "true" parameters) of up to 10% and still

the method can obtain the optimal parameters. We will present the true and estimated parameters for different data noise and different initial guess.

Keywords: smart materials, parameter estimation, optimization

CMPSD No. 5

ON CONNECTED GRAPHS THAT INDUCE THE INDISCRETE AND THE DISCRETE TOPOLOGIES

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There are various ways of constructing a topological space from a given graph G = (V(G),E(G)). Indeed, depending on the conditions imposed on some sets, one can generate a topological space from a given graph G = (V,E). Diesto and Gervacio have successfully given one construction of a topological graph. Their construction was further investigated by Guerrero, Canoy, and Lemence.

In this paper, we present a way of constructing a topology T(G) from a connencted graph G. In this type of construction, T(G) is the indiscrete topology on V(G) if and only if G is the trivial graph. We also characterized those connected graphs which induce the discrete topology. Specifically, we have obtained the following major results:

(1) Let G = (V(G),E(G)) be a connected graph. Then T(G) is the indiscrete topology on V(G) if and only if $G = K_1$.
(2) Let G = (V(G),E(G)) be a connected graph. Then T(G) is the discrete topology on V(G) if and only if for every a Î V(G) such that $D_2(a) \neq \emptyset$, the set $D_2(x) \cap [D_2(a) \cup \{a\}] \neq \emptyset$ for every x Î $D_2(a)$, where $D_2(a) = \{x \in V(G): d(x,a) = 2\}$.
(3) If K_n is the complete graph of order $n > 1$, then $T(K_n)$ is the discrete topology on V(G).
(4) If W_n is the wheel of order $n + 1$, where $n \geq 5$, then $T(W_n)$ is the discrete topology on V(G).

(4) Let C_n is the cycle of order $n^3 3$. Then $T(C_n)$ is the discrete topology on $V(C_n)$ if and only if $n^1 4,6$.

Keywords: connected graph, topology, base, indiscrete, discrete, complete graph, wheel, cycle

CMPSD No. 6a

SHADOWABILITY OF STATISTICAL AVERAGES IN A NONHYPERBOLIC CHAOTIC DYNAMICAL SYSTEM WITH UNSTABLE DIMENSION VARIABILITY: A SIMULATION STUDY

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Results of the study of Lai (1999) showed that the natural measure of a nonhyperbolic chaotic system can be related to the dynamical properties of all unstable periodic orbits embedded in part of a chaotic set contained in that region. Furthermore, he showed that at blowout bifurcation point there is a change in the transverse stability of an infinite number of unstable periodic orbits embedded in the chaotic attractor in the invariant subspace. Thus, for this system, the chaotic attractor becomes transversely unstable at this point. In effect, the natural measure of the chaotic attractor is unstable.

Motivated by this result, this research study investigated through simulation the stabilities and dynamics of statistical averages at blowout bifurcation point, a phenomenon in nonhyperbolic chaotic dynamical system with unstable dimension variability (UDV). which occurs when a chaotic attractor lying in some invariant subspace, becomes transversely unstable.In particular, the sensitivity of the mean and variance under various perturbations for the Henon type model was explored at the blowout bifurcation point.

The main conclusion of this paper is that systems having UDV are not statistically shadowable. The unstability of statistical averages has deep conse-

quences particularly in the validity of the model. As a result, there is a wide parameter regime for which the model does not accurately represent the deterministic evolution and statistical properties of the real system. Thus, no reliable information, deterministic or statistical, can be obtained.

Keywords: nonhyperbolic chaotic dynamical system, unstable dimension variability, natural measure, shadowability, blowout bifurcation point

CMPSD No. 6b

SPAN OF PARTITE GRAPHS

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A unit graph in the Euclidean n-space R^n is a graph whose vertices can be represented by points in R^n such that the distance between points representing adjacent vertices is equal to unity. If G is a unit graph in R^n and $\hat{G}$ is one such representation, then $\hat{G}$ is called a unit representation of G in R^n If is a unit representation of a graph G, then there is a smallest ball containing $\hat{G}$. The infimum of the diameters of these balls taken over all unit representations of G in R^n is called the span of G, denoted by $span_n G$.

For an n-partite graph G $span_{2n} \leq \sqrt{2(n-1)/n}$. If G is not empty, $span_n G$. for each $n \geq 4$. For the complete n-partite graph G, $span_{2n} \leq \sqrt{2(n-1)/n}$. For the complete bipartite graph $K(r,s)$, $span_4 K(r,s)$ is 1, 2, or $\sqrt{2}$ depending on n, r, and s.

Keywords: Euclidean space, unit graph, unit representation, ball, infimum, span, n-partite graph, complete n-partite graph

CMPSD No. 7a

ON THE HULL NUMBER OF THE COMPOSITION OF GRAPHS

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Given a connected graph $G = (V(G),E(G))$, the couple $(V(G), d)$, where $d(u,v)$ is the length of a shortest path connecting vertices u and v in G is a metric space on $V(G)$. Any u-v path of length $d(u,v)$ is called a u-v geodesic. A subset C of $V(G)$ is convex if for every two vertices u and v in C, the vertex set of every u-v geodesic is contained in C.

If u and v vertices of a graph G, then the set $I[u,v]$ is the closed interval consisting of u and v and all vertices lying on a u-v geodesic of G. If S then $I[S]$ is the union of $I[u,v]$, where u and v range over all elements of S. The convex hull $[S]$ of S is the smallest convex set containing S. It can be formed from the sequence $\{I^p[S]\}$, where p is a nonnegative integer, $I^0[S] = S$, $I[S] = [S]$, and $I^p[S] = I^{p-1}[S]$ for $p > 2$. For some p, we must have $I^p[S] = I^q[S]$ for all $q \geq p$. Further, if p is the smallest nonnegative integer such that $I^p[S] = I^q[S]$ for all $q \geq p$, then $I^p[S] = [S]$. A set S of vertices of G is called a hull set in G if $[S] = V(G)$ and a hull set of minimum cardinality is called a minimum hull set. The hull number of G, denoted by $h(G)$, is the cardinality of a minimum hull set in G.

In this paper, we give the hull number of the composition of two connected graphs. Among others, we obtained the following major results:

(1) Let G and H be connected graphs. If H is non-complete, then $h(G[H]) = h(H)$ if G is the trivial graph and $h(G[H]) = 2$ if otherwise.

(2) Let G be a connected graph and K_m be the complete graph of order m. Then $h(G[K_m]) = h(G) + (m-1)|A_e|$, where A_e is the set of extreme vertices of G.

(3) Let G be a connected graph of order $n > 3$ and K_m be the complete graph of order m. If G has no extreme vertices, then $h(G[K_m]) = h(G)$.

(4) Let G be a connected graph of order n and K_m be the complete graph of order m. If A_e (the set of extreme vertices of G) is a hull set in G, then $h(G[K_m]) = m|A_e|$.

Keywords: graph, geodesic, convex, convex hull, hull set, minimum hull set, hull number, composition of graphs

CMPSD No. 7b

ON TESTS OF MULTIVARIATE HYPOTHESES BASED ON THE ROOTS OF CERTAIN DETERMINANTAL EQUATIONS

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Multivariate tests in normal samples based on the roots of its associated matrix sometimes result in different tests. Quite a number of tests of hypothesis using maximum likelihood estimation (m.l.e.) and Union-Intersection (UI) approaches often result to the same test, but there are cases when they lead to different tests. From the nature of the determinantal equations resulting from both approaches, it is clear that functions of the roots of these equations are being used to represent the univariate analogue of variance 2; that is, det(*) and tr(*), the determinant and trace of the associated matrix (*). The difference thus arises due to the difference in the invariant measures of the matrix "structure" or configuration under test. In addition, both tests would be inadequate or insufficient in completely describing the structure. This paper proposes the use of the set of e.s.f (or trace statistics) tests to complete the structural tests on the associated matrix. Relevant distributional issues are discussed.

Keywords: multivariate test, associated matrix, determinantal equations

CMPSD No. 8a

ALTERNATIVE METHODS FOR SOLVING A TWO-DIMENSIONAL CARTESIAN TSUNAMI

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Abstract

In this paper, we formulate two alternative finite-difference methods for solving the system of partial differential equations describing a Cartesian tsunami in two-dimensions. In both methods, we will employ the explicit method for solving the parabolic partial differterential equation describing the variation of the vorticity with time. Furthermore we will use the Gauss-Seidel method for solving the elliptical partial differentiatial equation describing the stream function. The only difference between the two methods is that one will use a static grid and the other will use a dynamic grid. The formulation for the static grid with increments Δx and Δz (which correspond to the grid point coordinates x_i and z_j, respectively) do not vary in time. On the other hand, the formulation for the dynamic grid with increment Δx (corresponding to grid point coordinates x_i) do not vary in time; however, the increment Δz (corresponding to the grid point coordinates z_j) do vary in time. If we denote the velocity in the x and z directions by u and w, respectively, denote the pressure by p, and if we denote the density of the fluid by ρ, and viscocity by μ, then the laws of conservation of mass and momentum are given by:

The equation of continuity within the hydrosphere:

$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0$$

The equation of x-directed motion within the hydrosphere:

$$\rho\left[\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + w\frac{\partial u}{\partial z}\right] = -\frac{\partial p}{\partial x} + \mu\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial z^2}\right]$$

The equation of z-directed motion within the hydrosphere:

$$\rho\left[\frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + w\frac{\partial w}{\partial z}\right] = -\frac{\partial p}{\partial z} + \mu\left[\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial z^2}\right] - \rho g$$

The equation of continuity and motion at the ocean surface

$$\frac{\partial h}{\partial t} = w_h \, .$$

We will derive the governing equations given above, and also determine which of the two (alternative) methods yields better results.

Keywords: tsunami, finite difference, partial differential equations, law of conservation

CMPSD No. 8b

VERTEX COVER OF GRAPHS

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Let G be a graph. A set U of vertices in G is a vertex cover of G if every edge in G is incident with a vertex in U. The vertex covering number of G, denoted by $\alpha(G)$, is given by $\alpha(G) = \min\{|U| : U \text{ is a vertex cover of } G\}$. If H is a subgraph of G, then $\alpha(H) \le \alpha(G)$. For path P_n, cycle C_n, complete graph K_n, complete bipartite graph $K_{m,n}$, and Petersen graph P, we have, $\alpha(P_n) = \lfloor n/2 \rfloor$ $\alpha(C_n) = \lceil n/2 \rceil$ $\alpha(K_n) = n-1$, $\alpha(K_{m,n}) = \min\{m,n\}$, and $\alpha(P) = 6$.

Let $\bar{K}_n$ be the empty graph of order n. Then $\alpha(K_1 + G) = 1 + \alpha(G)$ and $\alpha(\bar{K}_n + G) = |V(G)|$ if $n \ge |V(G)|$. Moreover, $\alpha(\bar{K}_n + G) \le \min\{n + \alpha(G), |V(G)|\}$. It follows that $\alpha(\bar{K}_n + K_n) = n$, and $\alpha(F_{n,1}) \le \min\{n, n + \lfloor n/2 \rfloor\}$, where $F_{n,1}$ is the generalized fan and $W_{n,1}$ is the generalized wheel.

The following characterizations were also obtained: (a) characterization of vertex cover in terms of vertex independent set, (b) characterization of all graphs with vertex covering number equal to 1, and (c) characterization of hamiltonian complete bipartite graphs in terms of order and vertex covering number.

Keywords: graph, vertex cover, vertex covering number, independent vertices, hamiltonian graph

CMPSD No. 9a

NUMERICAL COMPUTATIONS OF TSUNAMIS THAT CAB BE GENERATED BY MANILA TRENCH EATHQUAKES

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This paper present numerical computations of possible tsunamis triggered by earthquakes in the Manila trench. In the study, different earthquakes scenarios were created at different points on the Manila trench and with varying fault parameters (such as magnitude, rupture direction of the fault plane. Etc.) of an earthquakes source model then compute the resulting tsunami amplitude for each scenario. This set of different scenarios were considered as a basis for the sensitivity analysis of tsunami wave characteristics near coastlines to identify earthquakes parameters that are most influential in tsunami generation from the Manila trench.

Linear and nonlinear conservation of momentum equation were used in the computations. The nonlinear terms can be neglected for propagation in deep ocean but should be retained for tsunami amplitude computation near the coast. The linear computation results for points near the coast is presented for comparison purposes.

This paper presents a preliminary investigation on the use of (linear and nonlinear) shallow water equations and a certain finite difference scheme in simulating tsunamis around the Manila trench/Manila bay area, we will not at this point concentrate on the applicability of numerical results to physical scenarios and cannot be used for emergency or mitigation planning. We believe this is the first attempt to numerically simulate earthquakes scenarios on this domain.

One limitation of this study is the unavailability of detailed bathymetry (ocean depth) data for the computational domain. We used the freely available Sandwell / Smith bathymetry from the internet. It has a 2-minute resolution (approximately 4km) and this is not enough for nonlinear computation near the shore.

Keywords: Tsunami, numerical computation, finite difference method, Manila Trench

CMPSD No. 9b

CONVEXITY AND A NON-CONNECTIVITY CONCEPT

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It is well known that the couple (V(G),d), where V(G) is the vertex set of a connected graph G and d(x,y) is the length of a shortest path connecting vertices x and y in G, is a metric space. Any x-y path of length d(x,y) is called an x-y geodesic. With this terminology, we say that a subset C of V(G), where G is a connected graph, is convex if for every two vertices x, y Î C, the vertex set of every x-y geodesic is contained in C.

We say that a nonempty subset S of V(G) is a non-connecting set in G if it satisfies the following condition: For every pair of vertices u, v Î V(G) \ S such that d(u,v) = 2, N(u) Ç N(v) Ç S = Æ. A non-connecting set with minimum cardinality is called a minimum non-connecting set. In this paper, we showed that if a set is convex set then its complement is a non-connecting set. Also, we characterized those subsets of V(G) that yield convex complements in V(G) using this non-connectivity concept. The main results obtained in this study are the following:

(1) Let G be a connected nontrivial graph. Then a minimum non-connecting set S in G is a singleton if and only if G has an extreme vertex.
(2) Let G be a connected graph and S a nonempty subset of V(G). If V(G) \ S is convex in G, then S is a non-connecting set in G.
(3) Let G be a connected graph of order n ³ 2. Then there is a convex set in G of order n - 1 if and only if a minimum non-connecting set in G is a singleton.
(4) Let G be a connected graph and S a nonempty subset of V(G). Then V(G) \ S is convex in G if and only if S is a non-connecting set in G satisfying the following property: (NN) For every nonempty non-singleton S* Í S and for any x, y Î V(G) \ S, S* is not contained in the vertex set of some x-y geodesic.

Keywords: graph, convex, geodesic, extreme vertex, non-connecting set, minimum non-connecting

CMPSD No. 10a

FOLDING THE SUM OF TWO GRAPHS

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The graph G' obtained from a connected graph G by identifying two nonadjacent vertices in G having at least one common neighbor is called a 1-folding of G. A sequence $G_0, G_1, G_2, \ldots, G_k$ of graphs such that $G_0 = G$ and G_i is a 1-folding of G_{i-1} for each $i = 1, 2, \ldots, k$ is called a k-folding of G. If G is not a complete graph, then it always has two nonadjacent vertices that have a common neighbor. Thus G can undergo a sequence of folding until a complete graph is obtained. Denote by F(G) the set of all non-isomorphic complete graphs that can be obtained from G by a sequence of folding.

This study attempts how to determine the smallest and largest element of F(G + H). It also tries to find a relationship between F(G + H) and F(G) + F(H). This study came up with the following conclusions:

1. Let G and H be two bipartite graphs. Then $K_4 \hat{I} F(G + H)$ and $K_4 = F(G) + K(H)$. Hence, $F(G+H)^{1} F(G) + F(H)$.
2. For any two graphs G and H each of diameter 2,
$$Kc_{(G+H)} \hat{I} [F(G + H) \text{Ç} (F(G) + F(H))].$$
3. For any graphs G and H, $F(H) + F(G) \hat{I} F(H + G)$.
4. For any graphs G and H, (a) $\max\{ s \mid K_s \hat{I} F(G + H)\} = q(G) + q(H)$, where q(G) and q(H) denote the maximum number into which V(G) and V(H) can be partitioned into independent and pairwise linked sets, respectively; and (b) $\min\{ r \mid K_r \hat{I} F(G+H)\} = p(G) + p(H)$, where p(G) and p(H) denote the minimum number into which V(G) and V(H) can be partitioned into independent and pairwise linked sets, respectively.

Keywords: 1-folding, k-folding, non-isomorphic, complete graphs, sum of two graphs, diameter, bipartite, independent, pairwise linked.

CMPSD No. 10b

ELECTRICAL CHARACTERISTICS OF POLYANILINE FILM AND THE n AND p – TYPE GERMANIUM CRYSTALS

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Numerous semiconductors already exist nowadays, may they be inorganic e.g. Ge and Si, or organic e.g. polyaniline and polythiophene semiconductors. The latter materials are of greater interests now because of their low cost synthesis and environmental stability. What signals their fundamental and practical applications are their magnetic, electronic and electrical properties that they exhibit in different temperature configurations especially at room temperature where most electrical and radiation devices such as rectifier diodes and EM wave absorbers, are operated.

In this study, electrical characteristics of n and p –type germanium crystals as well as the chemically prepared polyaniline films, an organic polymer, are investigated. Hall Effect experiments in conjunction with conductivity measurements via four – probe method are performed to measure the resistivity, charge carrier density and the hall mobility of each sample at room temperature. The respective resistivities of n and p –type germanium crystals are 8.10 ?.cm and 20.1?.cm with their corresponding charge carrier densities of 3.1×10^{14} cm^{-3} and 5.9×10^{15} cm^{-3}. The n – type shows a mobility of 2,477 $cm^2volt^{-1}.sec^{-1}$ and 1,825 $cm^2volt^{-1}.sec^{-1}$ for the p –type. On the other hand, the resistivity, charge carrier density and the mobility of the polyaniline samples are 3.41 ?.cm, 6.7×10^{14} cm^{-3}, 2,727 $cm^2volt^{-1}.sec^{-1}$, respectively.

Ohmicity of the current –voltage curve for all the samples is observed. The hall voltage of the germanium samples exhibit magnetic field dependence which is not observed in polyaniline samples. Applications of these samples such as radiation absorbers and sensors, particularly the polyaniline films, are under study.

Keywords: conducting polymer, polyaniline, resistivity, charge carrier density, mobility

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CMPSD No. 11

PREPARATION AND OPTIMIZATION OF ELECTRICALLY CONDUCTIVE FILMS: POLYPYRROLE OR POLYANILINE IN POLY(VINYL CHLORIDE) AND POLYSTYRENE

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Conducting polymers such as polyaniline (PAn) and polypyrrole (PPy) have poor physical properties, environmentally unstable and poor processibility. To obtain a mechanically stable film with high conductivity, conducting polymers are imbibed into the host polymers, poly(vinyl chloride) (PVC) and polystyrene (PS). This study aims to attain the optimum conditions to determine the highest possible conductivity with high mechanical strength which can serve as alternatives for metals used in aerospace application such as electromagnetic interference (EMI), shielding enclosures and spacecraft grounding.

Three composite films, PPy-PS, PPy-PVC and PAn-PVC, were studied which involves varying working conditions namely, the soaking time in the diffusion medium, the oxidation time, oxidant concentration and temperature. The monomers, pyrrole (Py) and aniline (An), were diffused into the base polymer matrices in the swelling medium of n-hexane and acetone mixture. The diffused monomer was oxidatively polymerized in a binary solvent system of acetonitrile and methanol in $FeCl_3$ for Py and $(NH_4)_2S_2O_8$ in HCl for An. The conductivity was measured using the four-point probe technique. Likewise, the tensile strength and the surface morphology via SEM were also conducted for further characterization.

The highest conductivity obtained was 1.33×10^{-2} Scm^{-1} for PPy-PVC (1 h monomer soaking, 0.8 M $FeCl_3$, 2.0 h oxidation at room temp), 1.75×10^{-3} Scm^{-1} for PPy-PS (8.0 min. monomer soaking, 1.0 M $FeCl_3$, 4.0 h oxidation at room temp) and 6.44×10^{-5} Scm^{-1} for PAn-PVC (10 min monomer soaking, 1.0 M $(NH_4)_2S_2O_8$, 2.0 h oxidation at room temp). The SEM analysis and the tensile strength tests are currently being undertaken.

Key words: conducting polymers, host polymers, polypyrrole, polyaniline, composite films

CMPSD No. 12

POLYANILINE FILM: PRODUCTION AND CHARACTERIZATION

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Conducting polymers are being extensively researched for their application in several new technologies. There is a lot of literature concerning the synthesis and characterization of conducting polymers. Examples of conducting polymers are polyaniline, polyacetylene, polypyrrole, and polythiopene. They have potential applications in electronic displays, as electrode materials in batteries, as molecular electronic circuit elements, in restoration of data, as indicators of gasometers and in biochemical analysis.

This study is on the production of a polyaniline film using the electrochemical polymerization method under potentiostatic conditions at room temperature. This method is done by supplying a constant voltage across the two electrodes (Indium Tin Oxide (ITO) and Platinum) that are immersed in an electrolytic solution containing aniline (monomer), hydrochloric acid (dopant), and distilled water (solvent). The resulting film is then characterized by measuring its conductivity and hall mobility using the Four Probe and Hall Effect apparatus. The current–voltage (I-V) characteristic curve of the film is also determined. In addition, the film produced is analyzed using the NIM and CAMAC instruments for performance testing.

Keywords: Conducting polymers, Polyaniline film, electrochemical polymerization, Nuclear Instrumentation Module (NIM), Computer Automated Measurement and Control (CAMAC), anilne, monomer, Four Probe and Hall Effect apparatus

CMPSD No. 13

PIEZOELECTRIC BIOMIMETIC SENSOR FOR DETERGENT BASED ON MOLECULARLY IMPRINTED POLYMER ELECTROSYNTHESIZED POLYPYRROLE

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Surfactants impose a great threat in the environment. There is therefore a need to monitor its concentration in water systems. Presently, the analytical methods used for the measurement of detergent require specialized personnel skill and expensive instruments. In this paper, we describe an alternative low cost and reliable method based on a piezoelectric biomimetic sensor.

The sensor involved a piezoelectric quartz crystal coated with a molecularly imprinted polypyrrole reagent phase. The reagent phase was electrosynthesized in the presence of pyrrole monomer and sodium dodecylsulfonate (SDS). In the presence of an applied potential, the monomer underwent polymerization and entrapped SDS molecules in its matrix. Equilibration with a buffer system resulted in the extraction of SDS, leaving behind cavities having a shape complementary to that of the template molecule. Upon exposure to a solution of SDS, the reagent phase re-binds template molecules within the cavities in its matrix.

The rebinding of SDS is monitored through measurement of the oscillation frequency of the quartz crystal. An instrumentation system was assembled based on a Pierce oscillator and a frequency counter. The preparation of the reagent phase was optimized by studying electropolymerization parameters such as time of polymerization, pH of buffer and current density. The resulting sensor exhibited a linear response to buffered SDS solutions containing from 10^{-7} M to 10^{-4} M SDS. It had an average response time of 2 minutes and showed a sensitivity of 38.223Hz/logM. The development of this biomimetic sensor, which uses artificial guest-host recognition systems, could provide an alternative strategy for anionic surfactant detection with consideration to cost, sensitivity, selectivity and ease of handling.

Keywords: Piezoelectric quartz crystal, molecularly imprinted polymer, sodium dodecyl sulfate, electropolymerization

CMPSD No. 14

MOLECULAR DESIGN OF MULTIVALENT SYNTHETIC VACCINES AGAINST BIOLOGICAL WARFARE (BW) AGENTS

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The new reality of biologic terrorism and warfare has ignited interests in the development, mass-production as well as dissemination of vaccines against BW agents to the general population, as the case of anthrax. One particular type of vaccine that possesses a strategic anti-terrorist advantage is the synthetic peptide vaccine. As an alternative to conventional vaccines, they are safe, they can be designed to induce defined immune responses and they can be synthesized in large quantities in high purity in a short span of time. In this study, we describe the molecular design of several candidate synthetic vaccines against the listed top BW agents of highest likelihood of rogue use, namely *Bacillus anthracis* (anthrax), smallpox, *Francisella tularensis* (tularemia), *Coxiella burnetti* (Q fever), *Yersinia pestis* (plague) and *Brucella melitensis* (brucellosis). Tapping into the huge genomic information available in the world wide web, candidate immunogenic peptides were engineered to create concatenated epitopes based on defined molecular criteria for T- and B-epitope prediction: proteosomal size and structural stability. The development of these BW vaccines represents a useful paradigm for the application of molecular bioinformatics and immunology into the defense arena.

Keywords: synthetic vaccines, biological warfare agents, protein engineering, epitopes

CMPSD No. 15

MOLECULAR ORBITAL CALCULATIONS ON THE MAILLARD REACTION: PROBABLE MECHANISM AND STRUCTURES OF INTERMEDIATES AND PRODUCTS

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The detailed mechanism of the Maillard reaction of sugars and amines leading to dark-colored polymeric (melanoidin) products has not been elucidated so far despite extensive kinetic and structural studies worldwide. Molecular orbital (MO) computation serves as a valuable tool in studying unstable reaction intermediates and in interpreting kinetic data, as well as in evaluating probable reaction mechanisms.

The present study deals with MO calculations on six Maillard reaction model systems consisting of glucose, fructose or xylose as sugar reactant and glycine or butylamine as amine reactant. The PM3 semi-empirical MO method was used to (a) calculate reactivities of reactants and probable intermediates, (b) evaluate molecular structures of polymeric products which have been suggested in the literature and (c) propose a polymerization pathway leading to melanoidin.

Ab initio, DFT and PM3 computations were performed on the sugar and amine reactants. Heats of formation (DH_f°) calculated using the PM3 method were closer to experimental values compared to ab initio and DFT results. Only PM3 computations were performed on molecular systems larger than the sugar or amine reactants. A computational level of accuracy of approximately 2.4 kcal/mol (0.02 kcal/g) was obtained using twenty organic compounds of known DH_f° values. All computations simulated molecular systems in vacuum. The computed HOMO-LUMO energy differences indicated that nucleophilic addition of two Amadori/Heyns rearrangement products is favored over combination with a sugar or amine.

The Yaylayan-Kaminsky (1998) polymeric product for the six model systems consistently gave the most negative computed values of DH_f° compared to the Kato-Tsuchida (1952) and Cammerer-Kroh (1995) products; the differences in DH_f° values among the proposed structures were greater than the estimated computational error. The computational results imply that the Yaylayan-Kaminsky mechanism is more probable than the Cammerer-Kroh and Kato-Tsuchida pathways.

Keywords: Maillard reaction, M.O. calculations, melanoidin, PM3

CMPSD No. 16

MOLECULARLY IMPRINTED ELECTRO-SYNTHESIZED POLY(O-PHENYLENEDIAMINE) BASED CAFFEINE SENSOR

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An investigation on the possibility of combining poly(o-phenylenediamine) as a sensing layer with molecular recognition capability for caffeine and piezoelectric quartz crystal was undertaken. The measurement of caffeine is necessary because of its occurrence in some of the food we eat and could pose as health hazards when taken in excessive amount.

The caffeine imprinted polymer was prepared using galvanostatic electropolymerization of o-phenylenediamine monomer directly onto one of the gold electrodes of a 9 MHz AT-cut quartz crystal. The optimum conditions including polymerization time, monomer to template ratio, current density and concentration of polymerizing solution during electro-synthesis of the reagent phase were considered. Extraction of the template caffeine from the polymer matrix was done by washing the polymer with water.

The instrumentation system for the caffeine sensor consists of a coated-quartz encased in a Teflon cell with its electrodes connected to Pierce-based oscillator circuitry and a frequency counter. Monitoring of the resonant frequency of the quartz crystal as it comes in contact with the caffeine solution was done in a stopped flow mode. A steady state response was achieved in about 10 min. The sensor exhibited a linear relationship between the frequency shift and caffeine concentration in the range of 0.1 to 10 mg/mL (correlation coefficient, r = 0.9923). It revealed a good sensitivity of about 130 Hz/ ln conc.(mg/mL) and good repeatability, rsd = 10.6 (n=7) for 0.5 mg/mL caffeine solution.

Surface examination of the sensor using scanning electron microscopy and x-ray photoelectron spectroscopy were also performed to have a better understanding of the sensor behavior and the imprinting process. The developed sensor can be used as a potential inexpensive option for measuring caffeine.

Keywords: Piezoelectric quartz crystal, molecularly imprinted polymer, caffeine, o-phenylenediamine

CMPSD No. 17

PREDICTION OF PROTEIN SECONDARY STRUCTURE USING TWO-LAYERED NEURAL NETWORKS

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In this study, prediction of protein secondary structure using two-layered neural network architectures was conducted.. Network training was performed using a data set of 126 globular proteins, which was in turn used for testing the 3-state (helix, sheet, and coil) predictive accuracy. To determine the network parameters at which optimum 3-state prediction occurs, predictive accuracy for a one-output node network was tested depending on the state threshold, the number of inputs used, and the number of hidden nodes used. Helix and sheet states were predicted most accurately (75% and 49%, respectively) with thresholds of 0.10 and -0.10, respectively, while for the coil state (99.9%) these were at 0.90 and -0.90, respectively. Helix and sheet predictions were found to generally increase with increasing number of inputs (76% and 53%, respectively) and hidden nodes (75% and 52%, respectively) used, while the opposite was true for coil prediction (26%). In addition, predictive accuracy for networks with one-output, two-output, and three-output nodes was compared. Overall accuracy increased with an increasing number of output nodes used (56% for the three-output network), but both helix and sheet prediction were better for the one-output node network (76% and 53%, respectively) while coil prediction was better for the two-output network (86%).

Keywords: neural network, secondary structure

CMPSD No. 18

A NEW ANALYSIS OF 6-JET HIGGSSTRAHLUNG CHANNEL AT JLC

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The Higgs boson H is a particle required by the Standard Model (SM) to explain many unanswered phenomena in Physics. At present, it is the only SM particle that has yet to be discovered by actual experiments, either directly or indirectly. This particle is known to be responsible for the mass generation of other particles through the process called Higgs Mechanism. None has been known exactly of this particle, not even its mass. In this paper, the decay width, $\Gamma(H \to X)$, or the standard deviation of the Higgs boson mass is studied by computer simulation of e^+e^- collisions in the proposed Asian Joint Linear Collider (JLC). JLC Study Framework (JSF) is employed for this experiment. JSF is a software library for the analysis of high energy physics data, based on the ROOT Data Analysis Framework. CERNLIB, ROOT, LCLIB libraries are also installed to be able to run JSF. The mass of the Higgs is assumed to be within the theoretical range of the SM. With this assumption of the Higgs mass, events of colliding electrons and positrons and their by-products can be generated using the PYTHIA Event Generator. Not only the target signal, $e^+e^- \to ZH \to q\bar{q}WW^* \to q\bar{q}q\bar{q}q\bar{q}$, but also the background signals which may mimic the desired signals and with considerable contributions. were also generated to determine the error of the measured quantity. Then the simulation of these events follows using the JSF Quick Simulator. The default configurations of the JLC detectors such as the different vertex detectors, central drift chamber, calorimeter, muon detector, and superconducting solenoid magnet are set before simulation. In the analysis of the data, the tracks found in the main detector are clustered to obtain the needed signals and then by formulating an event selection criteria further discrimination of unnecessary signals is done. So far obtained, we have calculated the relative error in Γ_{total} to be $\Delta\Gamma_{total}/\Gamma_{total} \approx 12$ percent. This is approximately equal to the square root of the target and background signals all over the target signals $\sqrt{S+B}/S$, from this we calculate the error. The discovery or non-discovery of the Higgs boson in a linear collider will change the course of our understanding of Physics. And if discovered, some theoretical predictions will be wiped out and some may

be strengthened by the determination of its mass alone. In fact, the existence of Higgs bosons might explain the possible beginnings of the universe and possibly uncover nano-technologies.

Keywords: Higgs boson, Standard Model, decay width, computer simulation, JLC Study Framework (JSF), Joint Linear Collider (JLC), CERNLIB, ROOT, LCLIB, PYTHIA Event Generator, JSF Quick Simulator

CMPSD No. 19

OPTIMIZATION OF SUPERCRITICAL CARBON DIOXIDE EXTRACTION OF THE ESSENTIAL OIL OF PHILIPPINE *Cananga odorata* Hook Fil et. Thomson FLOWERS BY RESPONSE SURFACE METHODOLOGY

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ABSTRACT

Essential oil was extracted from the flowers of Philippine Cananga odorata var. genuina grown in Pala-o, Iligan City by supercritical carbon dioxide (SC-CO2).

A statistical experimental design, first-order 2^3 factorial, was used to investigate the effects of three independent variables (pressure, temperature, and flow rate of CO2) on % oil yield (w/w), % linalool (v/v), and % benzyl benzoate (v/v) on the extracted oil. Three corresponding response equations have been generated for values of pressure (80-100 bar), temperature (35-50 °C) and flow rate of CO2 (1-4 mL/min). The pressure, temperature and flow rate of the SC-CO2 extraction conditions were 98.61 bar, 39.58 °C, and 2.99 mL/min, respectively. Gas chromatography was performed on the ilang-ilang oil extracted by SC-CO2, laboratory and commercial scale hydrosteam distillation. Two constituents of the

different ilang-ilang oils (linalool and benzyl benzoate) were evaluated with reference to the nature of the starting material, the extraction technique and source of plant material.

An optimum oil yield of 8.479 % (w/w) was obtained under the SC-CO2 extraction operating conditions. This oil yield is much higher compared to the oil yield from hydrosteam distillation which is 2-2.25 % (v/w). Degradation products were observed in hydrosteam distillation. On the basis of linalool to benzyl benzoate ratio, the SC-CO2 extraction of fresh flower (0.583) is much higher as compared to the SC-CO2 extraction of freeze-dried flower (0.009). The SC-CO2 extraction and hydrosteam distillation of freeze-dried sample gave a ratio of 0.009 and 0.001, respectively. The oil quality in Anao, Tarlac (0.658) is more superior than in Pala-o, Iligan City (0.583) due to the agroclimatic origin of the plant trees.

Keywords: benzyl benzoate; ilang-ilang oil; linalool; SC-CO2 extraction

CMPSD No. 20

GAMMA RAY SURVEYS FOR GEOLOGICAL STUDIES AND ENVIRONMENTAL MONITORING: EXPERIENCES AT THE PHILIPPINE NUCLEAR RESEARCH INSTITUTE

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ABSTRACT

The Philippine Nuclear Research Institute, with the assistance of the International Atomic Energy Agency, initiated the use of carborne and ground gamma ray survey techniques in lieu of the very expensive airborne survey. The objectives of this project were to establish environmental baseline information on the natural radioactivity of the entire country and to generate radioelement maps

for geological mapping and mineral resource assessment. In preparation of the planned nationwide survey, a regional survey was conducted over the small island of Marinduque (989 km^2) and a detailed survey was carried out at the San Antonio porphyry copper deposit in Sta. Cruz, Marinduque. Highlight of this study is the production of the first natural background radioactivity maps in the country. The radioelement maps in the regional survey showed good correlation with the local geology of Marinduque Island. Radiometric patterns in the detailed survey showing the combination of K and K/Th highs, including U and U/Th highs, if present, can be good radiometric-based indicators in the exploration for porphyry copper mineralization.

Carborne gamma ray spectrometric surveys were likewise undertaken at the former Subic US naval base and Clark US airforce base. This was due to mounting public concern over the presence of possible radioactive materials left behind by the US military forces in these bases. Using the gamma-ray spectrum ratio technique, results indicated the absence of radioactive sources in areas monitored within the two bases.

A sizeable part of Metro Manila was also covered by the carborne survey. Results discovered an area with high measurements of thorium up to 246.18 ppm. If converted to radiation dose would yield 5.88 mSv/y. This amount slightly exceeds the recommended maximum allowable radiation dose of 5 mSv/y that may be received by any individual. The radiation source comes from an establishment that produces mantles coated with thorium nitrate, a radioactive substance.

The surveys have demonstrated that the carborne and ground gamma ray spectrometric survey techniques are rapid and cost-effective.

Keywords: Environmental monitoring, carborne gamma ray survey, ground gamma ray survey, natural radioactivity, porphyry copper, radioelement

CMPSD No. 21

REMOVAL OF BASIC RHODAMINE B FROM AQUEOUS SOLUTION USING RICE STRAW AS ADSORBENT

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Rice straw, the leftover in rice grain harvesting, is a major agricultural problem because rice straws have poor biodegrability, and are generated in large amounts, 16 to 19 million metric tons in the year 2000. While some of the rice straws are used in mulching, as padding for egg transport, and as additive to animal feeds, a greater portion of rice straws is burned on the field.

In this study, we investigated the feasibility of rice straw as low-cost adsorbent for color removal of effluent from dyeing and textile finishing. The study focused on the removal of Basic Rhodamine B (BRB) from aqueous solution using rice straw as an adsorbent.

Results from batch equilibrium studies showed maximum sorptive capacities of rice straw for BRB are 22.5 mg/g and 15.5 mg/g at pH 2 and 12, respectively. Using the NAOH-H2O2 treated rice straw, the maximum sorptive capacities are 7.2 mg/g and 5.6 mg/g at pH 2 and 12, respectively. Delignification of the rice straw resulted in lower sorptive capacity for the basic or cationic dye such as BRB. This indicates that not only cellulose but also lignin and hemicellulose may provide significant active sites or functional groups that bind or adsorb cations from solution.

Results from column studies are consistent with the results observed in batch equilibrium studies. The bed reached its breakthrough and exhaustion time slightly earlier at pH 12 (compared to that of pH 2) and for NaOH-H2O2 treated rice straw (compared to that of untreated rice straw). The adsorption zone (D), bed sorptive capacity (N), and adsorption rate constant (K) were determined from the breakthrough profile. Results also showed that the initial dye concentrations and feed flowrates have significant effects on the adsorption behavior of BRB on the fixed bed of rice straws. The results from these studies will be useful for further researches in utilizing rice straw as an alternative adsorbent.

Keywords: rice straw, adsorption, Basic Rhodamine B, breakthrough curve

CMPSD No. 22

PARAMETRIC STUDY ON THE ADSORPTION OF BASIC RHODAMINE B ON SODIUM HYDROXIDE-PRETREATED CORN PITH

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Industries involved in dyeing operations discharge colored effluents. The color inhibits the penetration of sunlight through the surface of the receiving body of water, thus inhibiting the growth of photosynthetic organisms. In addition, some dyestuffs are potentially toxic to living organisms. In this study, we explored the potential of sodium hydroxide (NaOH) -pretreated corn pith as an adsorbent to remove Basic Rhodamine B (BRB) from aqueous solution. Corn pith is the soft and porous cellulosic part of cornstalk that is primarily used as animal feed in areas where there is extensive corn production.

Batch equilibrium experiments were conducted to investigate the adsorption of BRB from aqueous solutions on pretreated corn pith. Initially, the corn pith was pretreated at different levels of NaOH concentration (0.1M, 0.01M and 0.001M), pretreatment time (3 hours, 1 hour and 15 minutes), and pretreatment temperature (room temperature and 80°C).

The data were fitted to four different adsorption isotherm models (Langmuir, Freundlich, Redlich-Peterson and Brunauer-Emmet-Teller (BET)). The isotherms, which had average correlation coefficients greater than 0.97 were Langmuir, Freundlich and Redlich-Peterson respectively. The BET model had correlation coefficients less than 0.6.

Results indicated that the pretreatment of the corn pith resulted in the improvement of its adsorptive capacity for BRB. The maximum adsorptive capacities (Qmax) from the Langmuir model were determined for the different pretreatment conditions. Results showed that the Qmax of the pretreated corn pith ranges from 72.5- 105.0 mg/g. Pretreating the corn pith with 0.1 M NaOH at 80°C for 1 hour resulted to the highest improvement in the adsorptive capacity of corn pith, i.e., a 55.5% increase compared to that of untreated corn pith. On the other hand, the lowest in improvement was observed at pretreatment of corn pith with 0.001M NaOH at room temperature for 15 minutes i.e., a 7.25% increase compared to that of untreated corn pith. Statistical analysis of the data indicated that the effect of NaOH concentration, pretreatment time and temperature were significant (á = 0.05 level of significance). Results from this study will be useful for further optimization of parameters to maximize the adsorptive capacity of the pretreated corn pith.

Keywords: NaOH-pretreated corn pith, Basic Rhodamine B, adsorption isotherm

CMPSD No. 23

INVENTORY OF DIOXINS, FURANS AND DIOXIN-LIKE PCBs IN THE PHILIPPINES

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Emissions from polychlorinated dibenzo-p-dioxins (PCDD), polychlorinated dibenzofurans (PCDF) and dioxin-like PCBs which are formed unintentionally in industrial and combustion processes, were estimated through a Toolkit developed by United Nations Environment Program (UNEP) Chemicals. The Toolkit includes information on relevant industrial and non-industrial processes releasing PCDD/PCDF and detailed database of emission factors with default data representative of process classes. Screening matrix was applied to identify the main categories/subcategories of existing activities and sources in the country. Detailed information on the processes were gathered and classified. Releases were quantified using default/measured emission factors and estimates of the average annual release to air, water, land, products and residues were calculated by this basic equation: Source Strength (Dioxin emissions/year) = Emission Factor x "Activity Rate", presented in grams of toxic equivalents (TEQ) per annum (gTEQ/a).

Compiled PCDD/PCDF inventory yielded 530.70 gTEQ/a as total annual released to all environmental compartments. Uncontrolled combustion processes ranked 1st with 187.05 gTEQ/a followed by power generation/cooking at 157.23 gTEQ/a and production of chemicals and consumer goods at 91.56 gTEQ/a. Air had the highest PCDD/PCDF contamination with 327.60 gTEQ/a, product and land trailed with 77.64 and 46.86 gTEQ/a, respectively. Major source of PCDD/PCDF contamination for air and land was uncontrolled combustion of agricultural residues. This was in congruence with the study by United States Environmental Protection Agency (USEPA) that PCDD/PCDF released from open burning was higher compared to municipal solid waste incinerators. The Philippine waste incineration activity contributed only 6.7% of the total PCDD/PCDF released to the environment. Other major sources of PCDD/PCDF released

to products, water and residues were leather plants, open water dumping and household biomass cooking.

The Inventory could serve as guide in the formulation of National Action Plan for Persistent Organic Pollutants (POPs) as part of the country's obligation to the Stockholm Convention and basis for future exposure studies in PCDD / PCDF and dioxin-like PCBs.

Keywords: dioxins, furans, dioxin-like PCBs, national inventory, UNEP toolkit, TEQ

CMPSD No. 24

ANTIOXIDANT ACTIVITY AND TOTAL PHENOLIC CONTENT OF FRUITS AND VEGETABLES COMMONLY FOUND IN THE FILIPINO DIET

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Edible portions of 25 commonly eaten fresh fruits and vegetables in the Philippines listed into four groups namely, a) green leafy vegetables, b) other vegetables, c) root crops, and d) fruits, were analyzed for their antioxidant activity and total phenolic content. The antioxidant activity varied from 0 – 76%. Among the plant groups studied, root crops had the highest antioxidant activity, specifically 68.51% on the average. This is equivalent to more than 43.28-mg/g antioxidant activity of a - tocopherol. The total phenolic content of the fruits and vegetables studied range from 0 to 2015 mg catechin equivalents (CE)/100g sample.

Among the green leafy vegetable, kamote (Ipomea batatas) had the highest total phenolic concentration at 2015 mg CE/100g sample. Unripe jackfruit (Artocarpusheterophyllus), ubi (Dioscorea alata) and starapple (Chrysophyllum cainito) were the only plant foods in their group that showed considerable amounts of total phenolics with 807.5, 450, 502.5 mg CE/100g, respectively. Antioxidant activity and total phenolic content of the samples were not linearly correlated.

However, a strong significant correlation was observed when the samples were considered within a group.

The effect of processing and cooking, specifically boiling, on the antioxidant activity and phenolic content of the samples was also determined. Significant decreases in antioxidant activity were observed for jackfruit and gabi (Colocasia esculenta) at 41% and 37%, respectively. The total phenolic content of samples likewise decreased significantly. Boiling of root crops resulted in an average decreased of 30.6% in its antioxidant activity. On the other hand, the total phenolic content of both kamote and gabi was totally lost; but for ubi, a 22.9% decreased was observed. The activities of processed mango (Mangifera indica) and pineapple (Ananas comosus) were significantly greater than the fresh fruits. Blanching green leafy vegetables generally resulted in a significant decreased in antioxidant activity and total phenolic content.

Keywords: antioxidant activity, total phenols

CMPSD No. 25

ALKALOIDS FROM THE ANTITUBERCULAR FRACTION OF ALSTONIA SCHOLARIS (LINN.) R. BROWN LEAVES

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Tuberculosis is becoming a serious concern due to an upsurge of infected persons caused by the reemergence of multi-drug resistant strain of the causative agent, Mycobacterium tuberculosis. In the course of our study on the secondary metabolites from the antitubercular extracts of Alstonia scholaris (Linn.) R. Brown leaves, several indole alkaloids were isolated from the bioactive fraction of the alkaloid extract obtained at pH 5. This fraction exhibits a 99% inhibition to Mycobacterium tuberculosis H37Rv at 50 ug/mL using the Microplate Alamar

Blue Assay (MABA). The alkaloids were elucidated on the basis of the data obtained from UV, IR, mass spectrometry (LR-EIMS, LR-ESIMS, HR-ESIMS) and nuclear magnetic resonance spectroscopy (^{1}H, selective NOE, ^{13}C, APT, DEPT-90, DEPT-135, ^{1}H-^{1}H COSY, HMQC, HMBC, COLOC, ROESY). These were identified as, 19S-tubotaiwine, 6,7-secoangustilonine B and a new vallesamine indole alkaloid.

Keywords: Alstonia scholaris, indole alkaloids, Mycobacterium tuberculosis H37Rv, MABA

CMPSD No. 26

HYDROLYTIC ENZYMES FROM GERMINATING MUSTARD SEEDS (Brassica juncea): PURIFICATION, CHARACTERIZATION AND ENANTIOSELECTIVITY IN THE KINETIC REOLUTION OF RACEMIC a-ARYLPROPIONIC ESTER

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Hydrolases from germinating mustard (Brassica juncea) seeds were extracted with 0.1M Tris buffer containing 1 mM dithiothreitol. This was subjected to ammonium sulfate fractionation where the hydrolytic activity was found to be concentrated in the supernatant at 100% saturation; this fraction was passed through a hydrophobic interaction chromatographic column yielding a fraction with a purification factor of 185. The same fraction when passed through gel filtration column yielded a sample with 1370–fold increase in purification. Analysis through SDS–PAGE of active fractions revealed a common protein band at 41.2 kD.

The crude extract, the supernatant at 100% ammonium precipitation and the gel lipase active fractions were each used in the kinetic resolution of the racemic ester of an a-arylpropionic acid. All three fractions were found to be S (+) enantioselective where the product has 100% enantiomeric excess. Varietal difference indicated that the seeds from several sources exhibited distinct properties.

Keywords: hydrolases, enantioselectivity, mustard, Brassica juncea

CMPSD No. 27

PRODUCTION OF HIGH VALUE CHROMATOGRAPHIC SUPPORTS FROM LOCALLY AVAILABLE MATERIALS

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Chromatographic supports are of diverse nature depending on their intended application. These are made from an inert solid material to which is anchored active for resolution, catalysis and other uses. These supports are usually purchased abroad , are not manufactured locally and are therefore very expensive. This project hopes to circumvent this difficulty by producing chromatographic supports in the Philippines using locally available materials.

The Philippines, being a prime producer of sugar (sucrose) from sugar cane may increase the economic value of its products by converting sucrose into invert sugar. Invert sugar is 1.4 times sweeter than sucrose and is of great demand in the food and beverage industry. The suitable enzyme for conversion is invertase which may be immobilized on solid supports. Immobilization of the enzyme facilitates its conversion to a shelf reagent which is stable and reusable.

Chromatographic supports were prepared from locally available materials. Volcanic ejecta (lahar), chitosan, and nata de coco were used as solid support for the immobilization of yeast invertase and utilized for the conversion of sucrose to invert sugar. Some of the raw materials were converted to chemically active materials. The enzyme was immobilized by covalent bonding or adsorption on the solid support. Optimization of the immobilization procedures was conducted. The immobilized enzyme and solid supports produced were characterized to assess their performance. Experimental results indicated the efficiency and suitability of these materials as solid support. These studies could serve as ground work for the synthesis of chromatographic supports from locally derived materials for academic and industrial applications.

Keywords: chromatographic support, lahar, chitosan, nata de coco

CMPSD No. 28

THE PURIFICATION OF A PROTEASE FROM JACKFRUIT (Artocarpus heterophyllus) LATEX: ENANTIOSELECTIVITY OF ITS CATALYTIC ACTION IN THE HYDROLYSIS OF A METHYL ESTER OF A RACEMIC ARYPROPIONIC ACID

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A protease was extracted from jackfruit (Artocarpus heteophyllus) latex and purified to determine its potential as catalyst for the hydrolysis of 2–arylpropionic acid esters. The protein was localized in the precipitate of the 45% ammonium sulfate fraction (45 P). The fraction was desalted and subjected to ion exchange chromatography. A fraction was identified to be active and after SDS – PAGE analysis revealed the presence of a 22 and 27 kD protein bands.

The 45 P fraction was used to hydrolyze racemic ibuprofen methyl ester. HPLCX analysis using a chiral column indicated that the enzyme was at least 81% enantioselective for the hydrolysis of the R (-) methyl ester. This study demonstrated that the protease from jackfruit latex could be used for the preparation of R (-)-2 – arylpropionic acids.

Keywords: protease, enantioselective, jackfruit, Artocarpus heteophyllus