C2_C0244 SYNTHESIS AND CHARACTERIZATION OF $[Ru(bpy)_2(4mazpy)](NO_3)2.2H_2O$ COMPLEX

Dhassida Sooksawat[1], Kanidtha Hansongnern[1], Chaveng Pakawachai[2]

[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand. Email:kanidtha.h@psu.ac.th

Abstract: The complex of $[Ru(bpy)_2(4mazpy)](NO_3)_2.2H_2O$ (bpy = 2,2'-bipyridine, 4mazpy = 4-methyl-2-(phenylazo)pyridine) was synthesized and characterized. This compound was investigated by infrared spectroscopic and UV-Visible absorption spectroscopic techniques. In addition, the crystal structure of the complex was confirmed by single crystal X-ray diffraction method.

C2_C0253 CRYSTAL STRUCTURE OF THE 2:1 ADDUCT OF 1,2-BENZENEDIOL AND HEXAMETHYLENETETRAMINE

Kadsada Sala[1], Kenneth J. Haller[1], Seik Weng Ng[2]

[1] School of Chemistry, Suranaree University of Technology, Nakhon Ratchasima 30000 Thailand.

[2] Institute of Postgraduate Studies, University of Malaya, Kuala Lampur 50603 Malaysia. e-mail: kadsada@gmail.com

Abstract: The cocrystal product of an aqueous solution of 1,2-benzenediol (catechol) and hexamethylenetetramine (HMT) has been characterized by single crystal X-ray diffraction. The 2:1 product crystallizes in the monoclinic space group C2/c with one catechol and one-half HMT in the asymmetric unit. The crystal structure consists of sheets of HMT molecules at (1 1 0) with each HMT molecule located on a 2-fold axis through opposite methylene groups. Each HMT molecule is hydrogen bonded to four different catechol molecules by strong O–H···N hydrogen bonds. The catechol molecule exhibits one strong $R^1_1(5)$ intramolecular O–H O hydrogen bond ring, and links adjacent HMT molecules with $R^4_4(12)$ O–H···N hydrogen bonded rings, thereby creating two-dimensional sheets, and utilizing all the strong hydrogen bond donor and acceptor groups available. The two-dimensional sheets are linked into a three-dimensional network by weaker C–H π edge-to-face hydrogen bonds between 2_1-screw axes related catechol molecules stacked in herring-bone columns.

C3

C2_C0261 ENHANCEMENT OF CATALYTIC PERFORMANCE OF MCM-41 FROM RICE HUSK SILICA BY ADDITION OF TITANIUM

Surachai Artkla[1], Jatuporn Wittayakun[1], Nurak Grisdanurak[2]

[1] School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasrima, Thailand. E-mail:surachaiartkla@yahoo.com.

[2] Department of Chemical Engineering, Faculty of Engineering, Thammasat University, Pathumthani, Thailand.

Abstract: Mesoporous material, MCM-41, was synthesized by hydrothermal method from rice husk silica and modified further by adding titanium into its framework. The resultant solid product Ti-MCM-41 possessed high specific surface area and narrow pore size distribution. XRD pattern exhibited reflection of (100), (110) and (200) at 2θ lower than 10 degree and the form of loaded titanium was free-oxide titanium form. The Ti-MCM-41 was modified surface by KNO_3 and KOH and the resulting catalysts were designated as K/Ti-MCM-41 and K_2O/Ti-MCM-41, respectively. They were used to catalyze biodiesel production of palm olein oil and methanol via transesterification reaction. GC chromatograms showed that methyl palmitate, oleate and linoleate were clearly presented at retention time of 30.59, 41.36 and 45.40 min, respectively.

C2_C0262 SYNTHESIS OF ZEOLITE BETA FROM RICE HUSK SILICA AND UTILIZATION AS CATALYTIC SUPPORT FOR PLATINUM

Sittichai Kulawong, Sirinuch Loiha[1], Jatuporn wittayakun[1], Nurak Grisdanurak[2]

[1] School of Chemistry, Institute of Science, Suranaree University of Technology, Nakhon Ratchasrima, Thailand. E-mail:sake_ubu@yahoo.com

[2] Department of Chemical Engineering, Faculty of Engineering, Thammasat university, Pathumthani, Thailand.

Abstract: In this research, silica from rice husk was used in the synthesis of zeolite beta by hydrothermal method with the gel containing silica, alumina, sodium cation, tetraethylammonium hydroxide as a template, and water. The gel was transferred to a Teflon-linend autoclave and the crystallization of zeolite beta was done at 135 °C. The crystallization time was varied between 1 to 5 days and it was found that the minimum time to complete crystallization was 2 days. The zeolite beta structure was confirmed by X-ray diffraction analysis. Then platinum was loaded onto the zeolite surface by incipient wetness impregnation with a solution of platinum(II)acetate in acetone with the amount to give 1%Pt by weight. The catalyst was characterized by X-ray diffraction analysis and the zeolite beta was unchanged. The Pt/BEA catalyst was tested for carbon monoxide oxidation. It was found that the conversion was exponentially increased with increasing temperature. The maximum conversion reached 17% at 400 °C.

C3_C0008 MICROWAVE-ASSISTED ESTERIFICATION AND DIELS-ALDER REACTION OF SOME ESTERS AND ANTHRACENE ADDUCTS

Weerachai Phutdhawong[1]*, Duang Buddhasukh[2]

[1] Department of Chemistry, Maejo University, Chiang Mai, 50290, Thailand

[2] Department of Chemistry, Chiang Mai University, Chiang Mai, 50202, Thailand

Abstract: A facile, high yielding synthesis of 9,10-dihydro 9,10-ethano- anthracene-11-carboxylic acid methyl ester,

cis-9,10,11,15-tetrahydro-9,10[3',4']-furanoanthracene-12,14-dione, ethyl-p-nitrobenzoate, phenacetin and some related compounds using a modified commercial domestic microwave oven are reported

C3_C0009 KETONE GROUP BLOCKING AT THE C-20 POSITION OF STEROIDAL PROGESTIN INTERMEDIATES FOR MEDROXYPROGESTERONE ACETATE SYNTHESIS

Aranya Manosroi[1,2], Kaniana Rounto[2], Chonlada Komno[2], Penpan Khanrin[2] Aphiwat Teerawutgulrag[3], Duang Buddhasuk[3], Jiradej Manosroi[1,2]

[1] Faculty of Pharmacy, Chiang Mai University, Chiang Mai, Thailand 50200

[2] Natural Product Research and Development Center (NPRDC), Institute for Science and Technology Research and Development, Chiang Mai University, Thailand 50200.

[3] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand 50200

E-mail address: pmpti005@chiangmai.ac.th

Abstract: The objective of this study was to protect ketone group at the C-20 position of five steroidal progestins which were pregnenolone acetate (1), 17α-hydroxypregnenolone acetate (2), progesterone (3), progesterone acetate (4) and 17α-hydroxyprogesterone (5). Ethylene glycol was used as a blocking agent and the reaction was refluxed with toluene-p-sulphonic acid in benzene at 80 °C. The reaction was completed at 8 hours. The products were identified by IR in comparing with the standard intermediates, pregnenolone acetate 20-ethylene ketal (A); pregn-5-en-20-one, 3β, 17-dihydroxy-, cyclic ethylene acetal, 3-acetate (B) and pregn-5-ene-3,20-dione, 17-(acetyloxy)-, cyclic 3-(1,2-ethanediyl acetal) (C) which were the products of 1, 2 and 4 The %yield were 61.08%, 70.93% and 27.50% respectively. The intermediates 3 and 5 gave more than one product. Intermediate 3 gave 3 products of progesterone, cyclic 20-(ethylene acetal) (D); pregn-5-ene-3,20-dione, cyclic 3-(ethylene acetal) (E) and preg-5-ene-3,20-dione bis-ethylene ketal (F) with the %yield of 40.45%, 17.37% and 32.53% respectively, whereas 5 gave 3 products of pregn-4-ene-3,20-dione, 17-hydroxy-, cyclic 20- (ethylene acetal) (G) ; pregn-5-ene-3,20-dione, 17-hydroxy-, cyclic 3-(1,2-ethanediyl acetal) (H) and pregn-5-ene-3,20-dione, 17-hydroxy-, cyclic bis(ethylene acetal) (I) with the %yield of 22.06%, 1.93% and 9.42% respectively. This study has indicated that the acetoxy group at the C-17 position of 4 can hinder the reaction of ethylene glycol at C-20 position and the ketone group at the C-3 position of 3 and 5 can also react with ethylene glycol, thereby giving more than one product. Thus, 1 and 2 appeared to be the suitable steroidal progestin intermediates for the blocking process in the synthesis of medroxyprogesterone acetate (MPA)

C3_C0013 SYNTHESIS OF NOVEL AMORPHOUS HOLE-TRANSPORTING CARBAZOLE DENDRIMER

Vinich Promarak, Jirada Wajikamol and Phaoplrat Khasakeaw

Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, 34190, Thailand. E-mail address: pvinich@sci.ubu.ac.th.

Abstract: A novel amorphous hole-transporting carbazole dendrimer, 2,7-bis(3,6-di(carbazol-9-yl)carbazol-9-yl)-9,9-bis(n-hexyl)fluorene (**G2CF**), was synthesized by a divergent approach involving bromination and Ullmann coupling reactions. **G2CF** showed UV-Vis absorption bands at 304 and 332 nm in chloroform solution, and the photoluminescence spectra showed a maximum peak at 373 nm in a purplish blue region. Differential scanning calorimetry (DCS) and cyclic voltammetry (CV) revealed **G2CF** was an electrochemically and thermally stable amorphous material with a high glass transition temperature of 235 °C. The organic light-emitting devices prepared by spin-coating **G2CF** solution onto the indium-tin oxide (ITO)-coated glass substrate in conjunction with tris(8-quinolinolato)aluminum (Alq_3) and LiF/Al, as an electron transporting light-emissive layer and a metal cathode, respectively, showed a bright green emission with a maximum luminescence of 10,982 cd/m² at 16 V.

C3_C0014 SYNTHESIS AND CHARACTERIZATION OF TRIPHENYLAMINE CARBAZOLE-CAPPED MOLECULES

Vinich Promarak, Duangratchaneekorn Muenmart and Apinya Janpen

Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, 34190, Thailand. E-mail address: lumina125@hotmail.com

Abstract: A series of novel amorphous triphenylamine carbazole-capped molecules, 3,6-bis(3,6-bis(4-(diphenylamino) phenyl)carbazol-9-yl)-9-(2-ethylhexyl)carbazole (PACC) and 1,4-bis((3,6-di(4-(diphenylamino)phenyl)carbazol-9-yl)-3,6-di(2-ethylhexyloxy)benzene (PACB), was synthesized according to the divergent approach in which the desired molecules were built from the core outwards. The carbazole moieties were first connected to the brominated benzene and carbazole cores utilizing Ullmann condensation. Suzuki coupling reaction was employed to attach the triphenylamine units on the surface of the molecules. PACC and PACB showed UV-Vis absorption maximum at 330 and 336 nm in dichloromethane solution and the photoluminescence spectra showed a maximum peak at 401 and 393 nm in a purplish blue region, respectively. Cyclic voltammetry (CV) and differential scanning calorimetry (DCS) analysis revealed PACC and PACB were electrochemically and thermally stable amorphous materials with a high glass transition temperature of 187 and 121 °C, respectively. They are potentially blue light emitter or hole transporting layer for organic light-emitting devices.

C3_C0018 CHEMICAL CONSTITUENTS FROM THE LEAVES OF *Linostoma pauciflorum* Griff.

Tawesin Navarat [1], Songyos Pramjit[1] and Vatcharin Rukachaisirikul[2]

[1]Department of Chemistry, Faculty of Science and Technology, Songkhla Rajabhat University, Songkhla 90000, Thailand

[2]Department of Chemistry, Faculty of Science, Prince of Songkhla University, Songkhla 90112, Thailand

* Corresponding author. E-mail: ktaweesin@yahoo.co.uk

Abtract: Chemical investigation of the crude dichloromethane extract from the leaves of *Linostoma pauciflorum* Griff., upon chromatographic separation and purification, afforded two flavones (1 and 2) together with stigmasterol (3). The structures of these compounds were elucidated by analysis of 1D and 2D NMR spectroscopic data. Structure elucidation of other compounds are in progress.

C3_C0032 ELIMINATION OF PHORBOL ESTERS FROM JATROPHA CURCAS SEED OIL BY ADSORPTION

Rayakorn Nokkaew and Vittaya Punsuvon*
Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand.
E-mail: fscivit@ku.ac.th

Abstract: The seed oil of *Jatropha curcas* L. contains phorbol esters which is known as tumor promoting agent. Therefore it is necessary to find routes for detoxification. In this experiment, five adsorbents: activated carbon, diatomaceous earth, bentonite, chitosan, and chitin are used to adsorb phorbol ester at different time of adsorption. The result show that bentonite is the best adsorbent and it can adsorb the content of phorbol ester up to 98% in 45 minutes.

C3_C0033 ISOLATION AND DETERMINATION OF Δ9-TETRAHYDROCANNABINOL FROM *CANNABIS SATIVA L.* COLLECTED FROM MAETANG, CHIANG MAI

Pradudnate Katewong*, Kallaya PingMaung, Jirawan Banditpuritat, Napattarapong Suvannachai and Weerachai Phtdhawong
Department of Chemistry, Faculty of Science, Maejo University, Sansai, Chiang Mai, 50290 Thailand

Abstract: A procedure based on a common silica gel column chromatography was used for the isolation of Δ9-tetrahydrocannabinol from flowers, leave, trunks, roots and seeds of *Cannabis sativa L.* collected from Maetang, Chiang Mai. The elution solvent consisted of a mixture of hexane: toluene: acetone: acetic acid in a ratio of 65: 21.5: 13.5: 0.01 was used, which passed through the column at the flow rate 1.5 mL/min. The collected fractions were monitored by thin layer chromatography (TLC) which obtained 0.57 of the R_f value of Δ9-tetrahydrocannabinol. The maximal isolated yields were obtained about 0.50, 2.74, 0.49, 0.49 and 1.59 from flower, leave, trunk, root and seed, respectively. It was found that the THC quantity from flower is less than leave which is the opposited value comparing with the sample from the other area. The structural identification was confirmed using MS and IR by comparing with the database. The compound have 98% MS matching with the data base of National Institute of Standards and Technology(US) and the same retention time of GC chromatogram.

C3_C0037 Chemical Constituents from the Endophytic Fungus *Botryosphaeria mamane* PSU-M76

Wipapan Pongcharoen, Vatcharin Rukachaisirikul, Souwalak Phongpaichit, Nattawut Rungjindamai, Jariya Sakayaroj
[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand
[2] Department of Microbiology, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand
[3] National Center for Genetic Engineering and Biotechnology (BIOTEC), Thailand Science Park, Klong Luang, Pathumthani, 12120, Thailand

Abstract: The ethyl acetate extract from the broth of the endophytic fungus *Botryosphaeria mamane* PSU-M76, upon chromatographic separation, afforded one new benzodihydrofuran derivative (1), together with five known compounds [2,4-dimethoxy-6-pentylphenol (2), primin (3), (R)-(-)-mellein (4), *cis*-4-hydroxymellein (5) and *trans*-4-hydroxymellein (6)]. Their structures were elucidated by analysis of spectroscopic data, especially 1D and 2D NMR data. Among the isolated compounds, primin (3) exhibited the best antibacterial activity against standard *Staphylococcus aureus* ATCC25923 (SA) and methicillin-resistant *S. aureus* SK1 (MRSA) with equal MIC values of 38.4 μM.

C3_C0038 SYNTHESIS OF DERIVATIVES OF NAPHTHOQUINONE MONOOXIME AND THEIR CYTOTOXIC ACTIVITY

Chanya Chaicharoenpong[1], Songchan Puthong[1], and Tsutomu Ishikawa[2]*
[1] Institute of Biotechnology and Genetic Engineering, Chulalongkorn University, Bangkok 10330, Thailand.
E-mail:Chanya.C@Chula.ac.th, Fax: (662)2533543
[2] Graduate School of Pharmaceutical Sciences, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522, Japan.

Abstract: Chemical modification of naphthoquinone monooxime 5 was designed for investigating the new derivative with strong anti-tuomr activity. Derivatives of naphthoquinone monooximes 14 and 15 were synthesized and tested for cytotoxic activity against 5 human tumor cell lines. Compound 15 showed weak activity against human breast ductal carcinoma and human undifferentiated lung carcinoma and showed strong activity against human colon adenocarcinoma with IC_{50} 0.05 μg/ml, human gastric carcinoma with IC_{50} <0.001 μg/ml and human liver hepatoblastoma with IC_{50} <0.001 μg/ml.

C3_C0040 Chemical Constituents from the Unidentified Fungus PSU-SF13

Asadhawut Hiranrat[1], Vatcharin Rukachaisirikul[1], Souwalak Pongpaichit[2], Sita Predanon[2]
[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand
[2] Department of Microbiology, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand

Abstract: The ethyl acetate extract from the broth of the unidentified fungus PSU-SF13, upon chromatographic separation, afforded two new compounds; the dihydroramulosin derivative (2) and dechlorogriseofulvin derivative (7) together with five known compounds; dihydroramulosin (1), mellein (3), 4-hydroxymellein (4), griseofulvin (5) and dechlorogriseofulvin (6). Their structures were determined by analysis of spectroscopic data, especially 1D and 2D NMR data.

C3_C0055 Chemical Constituents from the Endophytic Fungus *Phomopsis* sp. PSU-D15

Ubonta Sommart, Vatcharin Rukachaisirikul, Souwalak Phongpaichit, Nattawut Rungjindamai, Jariya Sakayaroj
[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand
[2] Department of Microbiology, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand
[3] National Center for Genetic Engineering and Biotechnology (BIOTEC), Thailand Science Park, Klong Luang, Pathumthani, 12120, Thailand

Abstract: Investigation of the ethyl acetate extracts from the culture broth and cell of the endophytic fungus *Phomopsis* sp. PSU-D15 afforded one new amide derivative (1), together with five known compounds: the macrocyclic lactone (2), (1R,2S,4S)-mentanetriol (3), butanamide (4), uridine (5) and dicerandrol A (6). The structures were determined by analysis of spectroscopic data, especially 1D and 2D NMR spectroscopic data. The relative stereochemistry of 3 and 6 was established by analysis of NOEDIFF data.

C3_C0056 Chemical Constituents from the Unidentified Fungus PSU-SF5

Kongkait Trisuwan, Vatcharin Rukcahisirikul, Souwalak Pongpaichit, Sita Predanon
[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand
[2] Department of Microbiology, Faculty of Science, Prince of Songkla University, Hat Yai, Songkhla 90112, Thailand

Abstract: The ethyl acetate extract from the broth of the unidentified fungus PSU-SF5, upon chromatographic separation, afforded four new compounds; two furan derivatives (1 and 2) and two epoxydon derivatives (3 and 4), together with three known compounds; abscisic acid (5), deoxyabscisic acid (6) and epoxydon (7). Their structures were elucidated by analysis of spectroscopic data, especially 1D and 2D NMR data.

C3_C0062 A New Compound from Garlic with High Antioxidant Activity

Yongyuth Tundulawessa[1] Sinkan Pasook[2] Onjila Bouprasert[3]
[1] Department of Chemistry ,Faculty of Science , Srinakharinwirot University , Bangkok 10110
[2] Valaya Alongkorn Rajabhat University under Royal Patronage , Pratumtani Province
[3] Nakornpathom Rajabhat University, Nakornpathom Province

Abstract: The cinnamate (A) moiety was extracted form Garlic (*Allium sativum* L.) with methanol and partition by EtOAc. Purification by using column chromatography and recrystallization yielded the new white powder solid, mp 237-239°C (EtOH). This compound revealed antioxidant activity in DPHH and lipid peroxidant inhibition, results valued of IC_{50} 64.16 µg/mL and 2.8 mg/mL were higher than BHT and ascobic acid respectively.

C3_C0063 Chemical Constituents from the Twigs and Flowers of *Cratoxylum cochinchinense*

Suthida Rattanaburee and Wilawan Mahabusarakam
Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-yai, Songkhla 90112, Thailand.

Abstract: Air-dried twigs and flowers of *Cratoxylum cochinchinense* (Guttiferae) were extracted with dichloromethane. The crude dichloromethane extract of twigs and flowers were separated by chromatographic techniques and crystallization. Three known compounds: β-mangostin [1], mangostin [2] and 1,3,7-trihydroxy-2-(3-methyl-2-butenyl)-4-(3,7-dimethyl-2,6 octadienyl)xanthone [3] were obtained in twigs. The flowers afforded one new compound:3 - geranyloxy-1,7-dihydroxyxanthone [4], together with one known compound: 7-geranyloxy-1,3-dihydroxyxanthone [5] were yielded in flowers. Their structures were elucidated by analysis of spectroscopic data and comparison of the ^{1}H and ^{13}C NMR data with those reported previously.

C3_C0067 Chemical Constituents from the Root of Bruguiera cylindrica

Abdulwahab Salah Chanita Ponglimanont, Chatchanok Karalai.
Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand

Abstract: Three known diterpenoids and two triterpenoids : *ent*-kaur-16-en-13-hydroxy-19-al (1), 8,15R -epoxypimaran-16-ol (2), *ent*-kaur-9(11)-ene-13,17-epoxy-16-hydroxy-19-oate (3), lupeol (4) and betulinic acid (5) were isolated from the root of *Bruguiera cylindrica*.

C3_C0075 DIASTEREOSELECTIVE SYNTHESIS OF THE TRICYCLIC CORE OF SCHULZEINES

Sunisa Akkarasamiyo, Kritsada Atimanon, Punlop Kuntiyong
Department of Chemistry, Faculty of Science, Silpakorn University, Sanamchandra Palace Campus, Rajamanka Nai Road, Muang Nakhon Pathom, Thailand.
E-mail: niky_148@hotmail.com

Abstract: The tricyclic cores of a new class of marine natural products schulzeines have been synthesized in a short sequence using diastereoselective N-acyliminium ion cyclization as the key reaction. The N-acyliminium ion could be derived from treatment of α-hydroxy-δ-lactam with a Lewis acid. This intermediate in turn was prepared from 2-arylethylamine and L-glutamic acid derivative. The product of the key reaction, a tetrahydroisoquinoline fused with a δ-lactam, was obtained as an inseparable mixture of two diastereomers at C11b. The diastereomeric ratio was low and dependent on the Lewis acid used in the reaction. Trimethylsilyltrifluoromethanesulfonate gave the product with the diastereomeric ratio of 2.2:1 in favor of the 11b S diastereomer. Converting the N,N-dibenzyl derivative to the benzamide derivative enabled the separation of the two diastereomers by flash column chromatography.

C3_C0084 SYNTHETIC STUDIES OF C28 FATTY ACID SIDE-CHAIN OF SCHULZEINES

Nuanpan Piboonsrinakra, Ongard Nimpao, Punlop Kuntiyong
Department of Chemistry, Faculty of Science, Silpakorn University, Sanamchandra Palace Campus, Rajamanka Nai Road, Muang Nakhon Pathom, Thailand.
E-mail: nopknob@hotmail.com

Abstract: The studies toward syntheses of the C28 fatty acid side chains of schulzeines, a new class of marine natural products isolated from sponge *Penares schulzei*, have been carried out. In this ongoing research three subunits containing all 28 carbons of the fatty acids have been synthesized. The C1-C4 iodide was obtained from 1,4-butane diol in two straightforward steps. The C5-C17 portion was synthesized from 10-undecenoic acid. The C14-C15 bond was formed via Brown's enantioselective allylboration with the concomitant formation of C14 stereogenic center with the desired configuration. The C18-C28 fragment of the C28 fatty acid of schulzeine A was synthesized from 1-octanol. The C20-C21 bond formation was achieved by Brown's enantioselective diastereospecific crotylboration. In this step the C20 stereogenic center was formed with the methyl substituent in the desired configuration with high ee.

C3

C3_C0087 INTEGERRIMIDES A AND B: TWO NEW CYCLIC HEPTAPEPTIDES FROM THE LATEX OF *JATROPHA INTEGERRIMA*

Wolfgang Möller,[3] Harald Rösner,[3] Uwe Beifuss,[2] and Jürgen Conrad*,[2]
[1] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand, Institutes of [2]Chemistry and [3]Zoology, University of Hohenheim, Garbenstrasse 30, 70599 Stuttgart, Germany

Abstract: The investigation of chemical constituents have led to isolation of two new cyclic heptapeptides, integerrimides A and B (compounds 1 and 2) from the latex of *Jatropha integerrima* Jacq. Their structure elucidations were obtained by using extensive 1D and 2D NMR, MS and chemical degradation. Both peptides 1 and 2 at 50 µM inhibited to a certain degree cell proliferation of human ICP-298 melanoma cells, as well as cell migration of human Capan II pancreatic carcinoma cells, but both compounds were inactive in HSV-1, antifungal and antimalarial assays.

C3_C0089 NOVEL URSANE TRITERPENES FROM THE BARKS OF *DIOSPYROS DECANDRA*

Panchat Nareeboon[a], Wolfgang Kraus[b], Uwe Beifuss[b], Juergen Conrad[b], Iris Klaiber[b] and Somyote Sutthivaiyakit[a]*
[a] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, HuaMark, Bangkapi, Bangkok 10240, Thailand
[b] Institute for Chemistry, University of Hohenheim, Stuttgart 70599, Germany

Abstract: Novel 24-nor-, 24-nor-2,3-seco-, and 3,24-dinor-2,4-seco-ursane type triterpenes (1-5) have been isolated along with betulinic acid (6) from the stem bark of *Diospyros decandra*. The structures of these highly oxidized metabolites were elucidated by spectroscopic methods. Some isolates showed mild anti-mycobacterial activity against *Mycobacterium tuberculosis* with MIC values ranging from 25 to 200 µg/mL.

C3_C0091 CYTOTOXIC CARDENOLIDES FROM THE LEAVES OF CALOTROPIS GIGANTEA

Thitima Uhinhatrakool and Somyote Sutthivaiyakit
Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand

Abstract: Investigation of the CH_2Cl_2 extract of the leaves has led to the isolation of two new cardenolides, 19-*nor*-10-hydrocalactinic acid methyl ester (1) and 18,20-epoxycalotropin (2) together with 12 known compounds. The structural elucidation was accomplished by spectroscopic methods. Some of the isolates were evaluated for cytotoxic activity against KB, BC and NCI-H187 cancer cell lines, and all cardenolides tested were found to possess strong inhibitory effects. The presence of a deoxysugar at C-3, a formyl group at C-10, and an α,β-unsaturated-γ-lactone were crucial for cytotoxic activity.

C3_C0092 A CYTOTOXIC LIGNAN FROM THE ETHYL ACETATE EXTRACT OF *PHYLLANTHUS HULLETTII*

Saisuree Prateeptongkum[1] and Patoomratana Tuchinda[2]
[1] Department of Chemistry, Faculty of Science and Technology, Thammasat University, Khong-Luang, Prathumthani 12121, Thailand
E-mail:saisuree@tu.ac.th, Fax: (662)564-4483
[2] Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand.

Abstract: Chemical investigation of the ethyl acetate extract from aerial parts of *Phyllanthus hullettii* was performed by

column chromatography (CC) and recrystallization to yield glochidone (1), cleistanthin A (2). Their structures were elucidated by modern spectroscopic methods. Cleistanthin A (2) exhibited potent cytotoxic activities in several mammalian cancer cell lines, whereas glochidone (1) was inactive in all tested cell lines.

C3_C0094 Allelopathic and Antibacterial Activities of Organic Solvent Extracts from the Stem Bark of *Walsura trichostemon* Miq.

Pataranun Chotsang[1] Nuntana Aroonrerk[2] and Patchanee Charoenying[1]
[1] Department of Chemistry, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Bangkok 10520 Thailand
[2] Department of Stomatology, Faculty of Dentistry, Srinakharinwirot University, Bangkok 10110 Thailand
E-mail address: kcpatcha@kmitl.ac.th

Abstract: The effect of organic solvent extracts, after hexane ethyl acetate and methanol, from the stem bark of *Walsura Trichostemon* Miq. was investigated for their alleopathic and antibacterial activities. The allelopathic effect was tested against *Brassica campestris* var. chinensis L. (Chinese cabbage) seed germination and seedling growth. The crude ethyl acetate extract caused a decreased in the percentage of germination and shoot and root growth. Increasing concentration of the crude ethyl acetate extract resulted to higher inhibitory potential. In addition, the crude methanol extract was shown to have pronounced antibacterial effect against ten strains of gram-positive bacteria with MIC values in the range of 62.5-125 µg/mL).

C3_C0098 SYNTHESIS OF OPTICALLY ACTIVE GLYCIDYL ETHERS BY THE MITSUNOBU REACTION

Thanit Praneenararat, Tirayut Vilaivan*
Organic Synthesis Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Phayathai Road, Patumwan, Bangkok 10330, Thailand.

Abstract: Optically active glycidyl ethers were synthesized from glycidyl tosylate and glycidol via S_N2 reaction and the Mitsunobu reaction respectively. Both methods were compared in terms of percent yield and enantioselectivity of the products. Mitsunobu reaction was found to be a more effective method for the synthesis of these compounds.

C3_C0111 Chemical Constituents from the Stem of Caesalpinia pulcherrima

Virote Pranithanchai, Chatchanok Karalai[1], Sanan Subhadhirasakul[2].
[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand.[2]Department of Pharmacognosy and Pharmaceutical Botany, Faculty of Pharmaceutical Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand.

Abstract: Two known diterpenoids: isovouacapenol (1), 6β-cinnamoyl-7β-hydroxyvouacapen-5α-ol (2) and an homoisoflavonoid: bonducellin (3) were isolated from the stem of *Caesalpinia pulcherrima*.

C3_C0113 A DIRECT CATALYTIC ASYMMETRIC MANNICH-TYPE REACTION VIA A CHIRAL DINUCLEAR ZINC CATALYST

Jaray Jaratjaroonphong,[1,2,3] Vichai Reutrakul,[1] and Barry M. Trost[2]
[1] Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand.
E-mail: scvrt@mahidol.ac.th
[2] Department of Chemistry, Stanford University, Stanford, California 94305, USA.
[3] Current Address: Department of Chemistry, Faculty of Science, Burapha University, Chonburi 20131, Thailand.
E-mail: jaray@buu.ac.th

Abstract: An application of the chiral dinuclear zinc catalyst for the asymmetric synthesis of either *anti*- or *syn*-α-hydroxy-β-amino ketone had been investigated. In addition, the reactions focused on the use of α-hydroxyketones and enolizable imines. With the *N*-diphenylphosphinoyl(Dpp)-imine, the reactions were *anti* selective with ee's ranging from 83-99% except for the reaction of 2-methoxy-2'-hydroxy-acetylbenzene. On the other hand, with the *N*-Boc-imines, the reactions were *syn* selective with ee's from 90-94%. The dependence of the diastereoselectivity on the nature of the N-substituent presumably arises from the steric demands of the diphenylphosphinoyl group.

C3_C0114 SYNTHESIS OF PROLINAMIDE DERIVATIVES AS ORGANOCATALYSTS FOR ASYMMETRIC ALDOL REACTION

Sornpranart Sathapornvajana, Tirayut Vilaivan*
Organic Synthesis Research Unit, Department of Chemistry Faculty of Science, Chulalongkorn University, Phayathai Road, Patumwan, Bangkok 10330, Thailand.
*E-mail: vtirayut@chula.com

Abstract: Proline is a basic structural motif for many organocatalysts for asymmetric syntheses. In this work, prolinamide derivatives were synthesized from proline and 2-aminophenols in order to investigate their efficiency in catalysing asymmetric aldol reactions. A reaction between 4-nitrobenzaldehyde and cyclohexanone in the presence of the prolinamide derivative afforded the aldol condensation product with diastereoselectivity up to 9:1 and enantioselectivity over 90 %.

C3_C0125 SYNTHESIS OF 1,3-DIPYRENYL-CALIX[4]ARENE-CALIX[4]PYRROLE AS FLUOROGENIC SENSOR FOR ANION

Preecha Thiampanya and Buncha Pulpoka*
Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.
E-mail address: pre_274@yahoo.com, buncha.p@chula.ac.th

Abstract: 1,3-Dipyrenyl-calix[4]arene-calix[4]pyrrole (4) has been synthesized in 4 steps starting from calix[4]arene. The calix[4]pyrrole units were constructed through dipyrrole derivatives. After cyclization with acetone, the calix[4]pyrrole-calix[4]arene was coupled with *N*-(1-pyrenylmethyl)chloroacetamide to provide the desired product 4. The obtained products were characterized by spectroscopic techniques It is anticipated that the products could be used as a fluorogenic sensor for anions.

C3_C0137 SYNTHESIS OF SULFUR-CONTAINING CHIRAL LIGANDS FOR TRANSITION METAL-CATALYZED ASYMMETRIC NUCLEOPHILIC ADDITION TO CARBONYL COMPOUNDS

Woraluk Mansawat, Worawan Bhanthumnavin, and Tirayut Vilaivan*
Organic Synthesis Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
*e-mail address: vtirayut@chula.ac.th

C3

Abstract: Novel chiral ligands based on β-amino alcohols containing X as a soft donor atom (I) were synthesized and evaluated as ligands in transition metal-catalyzed asymmetric nitroaldol (Henry) reactions. Various reaction conditions for the Henry reaction have been studied (influence of ligand structure, temperature, molar ratio, solvent or type of metal). From preliminary study, chiral ligands containing thiophene could significantly catalyze nitroaldol reactions in high % ee. The reaction condition is simple and the stereochemical outcome is predictable from the configuration of the ligands.

C3_C0140 SYNTHESIS OF NOVEL CHIRAL AMINOALCOHOL LIGANDS FOR CATALYTIC ASYMMETRIC REACTIONS

Vorawit Banphavichit, Worawan Bhanthumnavin, and Tirayut Vilaivan*
Organic Synthesis Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
*e-mail address: vtirayut@chula.ac.th

Abstract: A series of N-salicyl-β-aminoalcohol ligands (I) had been synthesized by three-component Mannich type reaction followed by hydrolytic ring opening of the oxazolidine derivatives. The reactions provided novel chiral *N*-salicyl-β-aminoalcohol ligands (I) in high yields (84-92%) without any racemization. These synthesized compounds were evaluated as ligands for catalytic asymmetric Strecker reactions. The complexes prepared from ligands (I) and $Ti(O^iPr)_4$ are effective catalysts for catalytic asymmetric Strecker reactions. The reaction employing 10 mol% of catalyst provided the Strecker products in excellent yields and up to > 98% ee.

C3_C0151 ANTIMICROBIAL ACTIVITY OF 2-(1-ADAMANTYLTHIO) PYRIDINES

Supaluk Prachayasittikul[1], Chartchalerm Isarankura-Na-Ayudhya[2], Virapong Prachayasittikul[2] and Somsak Ruchirawat[3]
[1] Department of Chemistry, Faculty of Science, Srinakharinwirot University, Sukhumvit 23, Bangkok 10110, Thailand
[2] Department of Clinical Microbiology, Faculty of Medical Technology, Mahidol University, Bangkok-noi, Bangkok 10700, Thailand
[3] Laboratory of Medicinal Chemistry, Chulabhorn Research Institute, Vipavadee Rangsit Highway, Bangkok 10210, Thailand

Abstract: 2-(1-Adamantylthio) derivatives of 3-acetoxypyridine **1**, 3-ethoxypyridine **2**, and 5-pyridinol **3** were prepared. These 2-pyridyl sulfides, **1-3** were tested for antimicrobial activity against 24 strains of microorganisms using agar dilution method. It was revealed that compounds **1-3** inhibited the growth of β-hemolytic *Streptococcus* group A, α-hemolytic *Streptococcus*, and *Streptococcus* group D (enterococcus). The 5-pyridinol derivative 3 completely showed growth inhibition against β-hemolytic *Streptococcus* group A at 30 μg/mL.

C3_C0153 BIOTRANSFORMATION OF A NATURAL ENT-MANOYL OXIDE DERIVATIVE BY SOME FUNGI.

Somjintana Taveepanich[1], Robert Azerad[2], Michèle Maurs[2], and Amorn Petsom[3]
[1] Department of Chemistry, Faculty of Science, Ubonratchathani, Thailand, 34190.
[2] Laboratoire de Chimie et Biochimie Pharmacologiques et toxicologiques, URA 400 CNRS, 45 rue des Saints Pères, 75006-Paris, France.
[3] Research Centre for Bioorganic Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn University, Pathumwan, Bangkok, Thailand, 10330.

Abstract: The biotransformation of the labdane diterpene ent-1,2-dehydro-3-oxomanoyl oxide (**1**) (isolated from the stem bark of *Croton oblongifolius*) by *Rhizopus oligosporus*, *Rhizopus stolonifer* and *Mucor plumbeus* yielded three new metabolites, ent-11β-hydroxy-1,2-dehydro-3-oxomanoyl oxide (**2**), ent-(11β,14ξ,15)-trihydroxy-1,2-dehydro-3-oxomanoyl oxide (**3**) and ent-11β-hydroxy-3-oxomanoyl oxide (**4**). The structures of these metabolites were established on the basis of HRMS and 1D and 2D NMR spectral data.

C3_C0163 STATE OF THE ART FOR SYNTHESIS OF MOLECULARLY IMPRINTED POLYMERS

Virapong Prachayasittikul, Chartchalerm Isarankura-Na-Ayudhya,
Theeraphon Piacham, Somchai Boonpangrak, Chanin Nantasenamat, Thummaruk Suksrichavalit
Department of Clinical Microbiology, Faculty of Medical Technology, Mahidol University, Bangkok 10700, Thailand

Abstract: Molecularly imprinted polymers (MIPs) are macromolecular matrices that act as artificial receptors. In the early years, MIPs are prepared by the traditional bulk polymerization method and optimizations of the formulation have been performed empirically. In this study, we demonstrate the feasibility of using computer simulations for selecting optimal functional monomers in the formulation of MIPs, thereby speeding up the process of optimization The utilization of alternative polymerization method such as precipitation polymerization affords the production of uniformly-sized microspheres that are facile and affords better binding performance than the traditional bulk polymerization method. Precipitation polymerization yielded better binding performance than bulk polymerization as indicated from the selectivity index of 3.167 and 2.188, respectively. Furthermore, new initiators used for polymerization have also been shown to give better performance. This was observed from the selectivity index of 3.143 and 2.333, respectively, for polymers prepared by nitroxide initiator (3-(4-tert-butylphenyl)-1,1-dimethyl-3-(2,2,6,6-tetramethylpipendinooxy)propyl cyanide) and by the traditional benzoyl peroxide initiator. Moreover, we have also demonstrated the feasibility of using surface bound photo-radical initiators (2,2'-Azobis(2-amidinopropane) hydrochloride) for the synthesis of MIP films with controlled thickness of < 50 nm on QCM surface. The sensor generated a large frequency change (>30 Hz) upon encountering a small amount of analyte. It also displayed short response time (<1 min) as well as possessing chiral selectivity towards the template molecule at a concentration higher than 0.38 mM, in aqueous solution. The combined use of these methodologies has great implications for preparing MIPs with enhanced and robust performance.

C3_C0167 COMPUTATIONAL INSIGHTS OF SULFONAMIDE IMPRINTED POLYMERS

Chartchalerm Isarankura-Na-Ayudhya[1], Chanin Nantasenamat[1], Prasit Buraparuangsang[1,2], Theeraphon Piacham[1,2], Leif Bulow[2], Lei Ye[2], Virapong Prachayasittikul[1]
[1]Department of Clinical Microbiology, Faculty of Medical Technology, Mahidol University, Bangkok 10700, Thailand
[2]Pure and Applied Biochemistry, Chemical Center, Lund University, Box 124, 22100 Lund, Sweden

Abstract: Molecular imprinting is one of the most efficient methods for preparing synthetic receptors possessing user defined recognition properties. Despite general success of non-covalent imprinting for a large variety of templates, some groups of compounds remain difficult to tackle due to their structural complexity and poor solubility. In this study, we investigated preparation of molecularly imprinted polymers which can bind several sulfonamide compounds representing important drug candidates. Compared to the biological system that utilizes metal coordinated interaction, the imprinted polymers provided pronounced selectivity when hydrogen bond interaction was employed in an organic solvent. Computer simulation of the interaction between sulfonamide template and functional monomers pointed out that 1-vinylimidazole (VIM) was optimal for imprinting sulfonamides that coincided with the experimental results.

C3_C0177 EFFICIENCY OPTIMIZATION OF THE SYNTHESIS OF POLYTHIOPHENE DERIVATIVES

Ketthip Anuwareephong[a], Worawan Bhanthumnavin[a,b], Yongsak Sritana-anant[a,b]
[a] Program of Petrochemistry and Polymer science, Faculty of Science, Chulalongkorn University;
[b] Department of Chemistry, Faculty of Science, Chulalongkorn University; Tel:02-218-7632

Abstract: The oxidative coupling of thiophene monomer with anhydrous ferric chloride in organic solvent is one of the prefered methods to synthesize polythiophene and its derivatives. This research investigated the various experimental factors in the polymerization reaction to yield poly(3-hexylthiophene) including reaction temperature, mole ratios of 3-hexylthiophene and ferric chloride, types of solvent and additives, with the goal of reaching to obtain highest %yield and Head-to-Tail ratio (%HT). The best condition for the synthesis of poly(3-hexylthiophene) was found when running to the reaction at room temperature in dichloromethane and at mole ratio of 3-hexylthiophene monomer : ferric chloride = 3:9. Under this condition, the polymer was obtained in 94%yield with 78% HT. Decreasing the reaction temperature slightly raised %HT, however, the %yield was lower. In the case of the influence of the additives, water was found to decrease %HT of the resulting polymer. Among the other tested solvents, dichloroethane was the best choice gave comparable result to those of dichloromethane, yielding 94% of poly(3-hexylthiophene) with 73% HT.

C3_C0179 SYNTHESIS OF POLYESTER CONTAINING *P*-ALKOXYCINNAMATE

Pruetinan Changhin[1], Yongsak Sritana-anant[1,2], Supason Wanichweacharungruang[1,2]
[1] Department of Petrochemistry and Polymer Science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.
[2] Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.

Abstract: Three polymers containing UV absorptive chromophore were synthesized from the following monomers: 1,2(bis(4-(2-carboxyvinyl)phenoxy))ethane (M2) and 1,12(bis(4-(2-carboxyvinyl)phenoxy))dodecane (M12). The syntheses of three polymers were done through condensation polymerization between M2 or M12 and poly(ethylene glycol)200 (PEG200) or poly(ethylene glycol)400 (PEG400).[1,2] Molecular weights of all three polymers were in the range of 1500-6000. Absorption profiles of all synthesized polymers indicated UV-B absorption property. In addition, the synthesized copolymer between M2 and PEG400, a yellowish liquid, showed good solubility in various organic solvents. With the desired characteristics, namely high molecular weight, UV absorption properties and solubility properties, the polymers will be tested for cosmetic application

as potential UV filters with minimal transdermal penetration.[3,4]

C3_C0183 SYNTHESIS OF POLY(2-ETHYLHEXYL CINNAMATE-4-VINYL ETHER) AND POLY(DIALKYLBENZALMALONATE-4-VINYL ETHER)

Rattanan Tuangudomsap[1], Supason Wanichweacharungruang[2]
[1] Program of Petrochemistry and Polymer Science, Faculty of Science, Chulalongkorn University, Phyathai Road, Bangkok 10330, Thailand.
[2] Department of Chemistry, Faculty of Science, Chulalongkorn University, Phyathai Road, Bangkok 10330, Thailand.

Abstract: Octyl methoxycinnamate (OMC), the most widely used sunscreen agent in various cosmetic formulations, although shows only few allergic reactions to human skin, its transdermal permeation into human body and its low photostability have also been realized.(1-3) To solve both transdermal absorption and photostability problems, polymers of cinnamate and benzalmalonate derivatives, poly(2-ethylhexyl cinnamate-4-vinyl ether) and poly(dialkylbenzalmalonate-4-vinyl ether) were synthesized in this research.(4) The poly(diethylbenzalmalonate-4-vinyl ether) obtained by a radical polymerization with the number-average molecular weight (M_n) of 1900-2000 showed UVB (290-320 nm) screening properties.

C3_C0191 CHITOSAN-NANOPARTICLES AS CARRIERS FOR COSMETIC ACTIVES.

Nattaporn Anumansirikul[1], Supason Wanichweacharungruang[2], Suwabun Chirachanchai[3]
[1] Program of Petrochemistry and Polymer Science, Faculty of Science, Chulalonghorn University, Phyathai Road, Bangkok, Thailand 10330;
[2] Department of Chemistry, Faculty of Science, Chulalongkorn University, Phyathai Road, Bangkok, Thailand 10330;
[3] The Petroleum and Petrochemical College, Chulalongkorn University, Phyathai Road, Bangkok, Thailand 10330.

Abstract: In this work, chitosan-nanoparticles were obtained directly from the reaction of N-phthaloylchitosan and methoxy poly(ethylene glycol) methyl ether terminated carboxylic group. The products are stable white particles with the average sizes of about 40-150 nm as shown by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). These chitosan-nanoparticle can be loaded with various cosmetic active ingredients such as octyl methoxycinnamate (OMC), ascorbyl palmitate (vitamin C derivative) and astaxanthin.

C3_C0193 Synthesis of bipyridyldiporphyrin as photosensitized dye for organic solar cell

Preeyanut Duangtaor and Buncha Pulpoka*
Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.
E-mail address: ppreeyanut@hotmail.com, buncha.p@chula.ac.th

Abstract: Bipyridyldiporphyrin (**6**) has been synthesized in 6 steps starting from 4,4'-dimethylbipyridine. The first 4 steps concerned the transformation of 4,4'-dimethyl bipyridine to 4,4'-diformylbipyridine. The fifth step involved the preparation of a tetrapyrrane (**5**) which was condensed with **4** in refluxing propionic acid/toluene using air-oxidation to provide bipyridyldiporphyrin (**6**). The obtained product was characterized by spectroscopic techniques and aimed to be used as a photosensitized dye in organic solar cell.

C3_C0208 CONSTRUCTION OF MOLECULARLY IMPRINTED POLYMERS FOR CHOLESTROL BY SEMICOVALENT IMPRINTING APPROACH AND NITROXIDE MEDIATED RADICAL POLYMERIZATION

Somchai Boonpangrak[1], Virapong Prachayasittikul[1], Michael J. Whitcombe[2], Klaus Mosbach[3], Lei Ye[3]
[1] Department of Clinical Microbiology, Faculty of Medical Technology, Mahidol University, Bangkok, Thailand
E-mail address: mtvpr@mahidol.ac.th, Fax: (662) 849-6330
[2] Institute of Food Research, Norwich Research Park, Colney, Norwich NR4 7UA, UK
[3] Pure and Applied Biochemistry, Chemical Centre, Lund University, 22100 Lund, Sweden

Abstract: The use of molecularly imprinted polymers (MIPs) in chemical and bioanalytical applications has been gaining in interest in recent years. Compared to their biological receptor counterparts, MIPs are easy to prepare, have long shelf stability and can be used under a variety of harsh conditions. The majority of MIPs currently used are produced by traditional free radical polymerization. One drawback with the use of standard free radical initiators is that little control can be exerted over the chemical processes that form the final imprinted cavities. In this study we set out to investigate the application of controlled (living) free radical polymerization to the preparation of MIPs. This was exemplified by the synthesis of cholesterol-imprinted bulk polymers by nitroxide-mediated polymerization (NMP). A sacrificial covalent bond was employed to maintain imprinting fidelity at elevated temperature. Selective uptake of cholesterol from solutions in hexane was studied with imprinted polymers prepared under different conditions. The imprinted hydrolyzed MIP prepared b NMP displayed higher selective cholesterol binding than that prepared by a traditional radical polymerization.

C3_C0211 REACTION OF SOME 4,6-DIMETHOXYINDOLES WITH NITRIC ACID: NITRATION AND DIMERISATION

Tinnagon Keawin[1], Shuleewan Rajviroongit[2] and David StC. Black[3]
[1] Department of Chemistry, Faculty of Science, Ubon Ratchathani University
Warinchumrap, Ubon Ratchathani 34190, Thailand.
[2] Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand.
[3] School of Chemistry, The University of New South Wales, UNSW Sydney, NSW 2052, Australia

Abstract: A range of 3-aryl-4,6-dimethoxyindoles bearing electron-withdrawing groups in at either the C2- or C7-position can be nitrated using nitric acid in acetonitrile, to give 7-nitro or 2-nitro-indoles, respectively. Those without electron-withdrawing groups undergo oxidative dimerisation either at C7, if they are 2,3-disubstituted, or at C2, if they are N-methylated and unsubstituted at C2.

C3_C0212 ALKALOIDS FROM CRUDE METHANOL EXTRACT OF ROOTS OF *POLYALTHIA CERASOIDES*

Ratsami Lekphrom, Somdej Kanokmedhakul, and Kwanjai Kanokmedhakul
Department of Chemistry, Faculthy of Science, Khon Kaen University, Khon Kaen, 40002, Thailand.

Abstract: Chromatographic separation of the crude MeOH extract of roots of *P. cerasoides* led to the isolation of four isoquinoline alkaloids; laudanosine (**1**), codamine (**2**), laudanidine (**3**) and reticuline (**4**). The structures of these compounds were identified by spectroscopic methods. Bioactivity assays revealed that compounds 2 and 3 showed activities against malalia with IC_{50} values of 4.24 and 7.02 µg/mL, respectively.

C3_0214 CHEMICAL CONSTITUENTS FROM CRUDE HEXANE AND EtOAc EXTRACTS OF *EMERICELLA NIDULANS*

Panawan Moosophon[1], Somdej Kanokmedhakul[1], Kwanjai Kanokmedhakul[1], and Kasem Soytong[2]
[1] Department of Chemistry, Faculty of Science, Khon Kaen 40002, Thailand.
[2] Department of Plant Pest Management Technology, Faculty of Agricultural Technology, King Mongkut's Instituente of Technology Ladkrabang, Bangkok 10520, Thailand.

Abstract: Chromatographic separation of the crude hexane extract from *Emericella nidulans* led to the isolation of five compounds, epishamixanthone (**1**), shamixanthone (**2**), emericellin (**3**), ergosta-6, 22-diene-3-ol-5, 8-epidioxy-(3β- 5α, 22E) (**4**) and sterigmatocystin (**5**), while the ethyl acetate extract gave one compound, demethylsterigmatocystin (**6**). The structures of the isolation compounds were identified by spectroscopic method.

C3_C0220 STEREOSPECIFIC SYNTHESIS OF 1,2-CIS GLYCOSIDES *VIA* VINYL-MEDIATED INTRAMOLECULAR AGLYCON DELIVERY (IAD)

Kamoanart Chavajarus[1] and Antony J Fairbanks[2]
[1] Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Warinchumrap, Ubon Ratchathani 34190 Thailand
[2] The Chemical Research Laboratory, University of Oxford, Mansfield Road, Oxford OX1 3TA, UK

Abstract: Stereospecific synthesis of 1,2-*cis* glycosides *via* vinyl-mediated intramolecular aglycon delivery (IAD) had been studied. Tethering reactions of 2-*O*-vinyl thioglycosides, synthesized from the corresponding 2-*O*-unprotected glycosyl donors by Ir-catalyzed transvinylation with vinyl acetate, and a range of glycosyl acceptors were achieved by using I_2/AgOTf/CH_2Cl_2 in the presence of a hindered base 2,6-di-*tert*-butyl-4-methyl pyridine (DTBMP). Subsequent activation of the resulting mixed acetals with I_2/AgOTf/DTBMP in acetonitrile furnished the desired 1,2-*cis* α-*gluco* and β-*manno* pyranosides in a completely stereoselective fashion *via* an intramolecular glycosylation. In addition, attempted one-pot intramolecular glycosylations were also investigated. The desired 1,2-*cis* glycosides were unfortunately isolated in lower yield than those produced by the two-step process.

C3_C0247 SOLID PHASE SYNTHESIS OF POLYAMINES-DIHYDROCAFFEIC ACID CONJUGATES AND THEIR ANTIBACTERIAL ACTIVITY AGAINST DRUG-RESISTANT STRAINS

Nuttapon Apiratikul[1], Boon-ek Yingyongnarongkul[1]*, Nuntana Aroonrerk[2] and Apichart Suksamrarn[1]
[1] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand;
e-mail address: boonek@ram1.ru.ac.th
[2] Department of Stomatology, Faculty of Dentistry, Srinakharinwirot University, Watana, Bangkok, 10110.

Abstract: Hydroxycinnamic acid amides (HCAAs) (e.g., 4-hydroxycinnamoyl putrescine) are widely distributed in higher plants and might pay a role in the chemical defense of plants against bacterial and fungal pathogens. It has been shown that dihydrocaffeoyl analogues of diamines exhibited antibacterial activities against MRSA and VRSA. This work deals with the solid phase synthesis of HCAAs using polyamines core containing two, three and four dihydrocaffeoyl groups. Some of these compounds showed higher antibacterial activity against MRSA and VRSA than the diamines analogues.

C3_C0248 EFFECT OF SPACER LENGTH OF CATIONIC LIPIDS FOR DNA DELIVERY

Puchanee Lamulsuk[1], Boon-ek Yingyongnarongkul[1]*, Ramida Watanapokasin[2], and Apichart Suksamrarn[1]
[1] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand;
e-mail address: boonek@ram1.ru.ac.th,
[2] Department of Biochemistry, Faculty of Medicine, Srinakharinwirot University, Bangkok, 10110.

Abstract: Cationic lipids are non-viral vector to deliver oligonucleotide/DNA into the cells. The multi steps nature of the transfection pathway has made it very difficult to study structure-activity relationships of transfection compounds. It was thus necessary to have an empirical approach, which involves the use of combinatorial library approach to achieve high advantage in the study. The present work deals with the synthesis of cationic lipids with different spacer using solid phase technique. The optimum spacer between cationic head and hydrophobic tail to give highest transfection efficiency was 4 carbon atoms.

C3_C0249 BIOTRANSFORMATION OF 20-HYDROXYECDYSONE 2-MESYLATE TO 3-DEHYDRO-2-DEOXY-ANALOGUES BY CURVULARIA LUNATA NRRL 2178

Chatchawan Changtam[1], Oratai Sukcharoen[2], Boon-ek Yingyongnarongkul[1] and Apichart Suksamrarn[1,*]
[1] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand; [2]Department of Biotechnology, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand;
e-mail address: curcumin1@yahoo.com

Abstract: 20-Hydroxyecdysone 2-mesylate (1), was biotransformed to the rare ecdysteroid, 3-dehydro-2-deoxy-20-hydroxyecdysone (2), by the fungus Curvularia lunata NRRL 2178. Ponasterone A 2-mesylate (3), pterosterone 2-mesylate (5) and shidasterone 2-mesylate (7) were similarly biotransformed to the corresponding 3-dehydro-2-deoxy-analogues.

C3_C0250 MICROBIAL HYDROXYLATION AND REDUCTION OF DIBENZALACETONE BY CURVULARIA LUNATA AND CUNNINGHAMELLA ECHINULATA

Marneerat Sagamenjit[1], Chatchawan Changtam[1], Oratai Sukcharoen[2], Boon-ek Yingyongnarongkul[1] and Apichart Suksamrarn[1,*]
[1] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand;
e-mail address: apichart@ram1.ru.ac.th;
[2] Department of Biotechnology, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand

Abstract: 1,5-Diphenylpenta-1,4-dien-3-one (1) (dibenzalacetone) was biotransformed to 1,5-diphenylpentan-3-one (2), 3-hydroxy-1,5-diphenylpentane (3) and 3-hydroxy-1-(4-hydroxyphenyl)-5-phenylpentane (4) by Curvularia lunata NRRL 2178 the latter of which was difficult to obtain by chemical means. Biotransformation of 1 with Cunninghamella echinulata NRRL 1386 produced 2, 3 and 1-hydroxy-1-(4-hydroxyphenyl)-5-phenylpentan-3-one (5).

C3_C0251 THE CHEMICAL CONSTITUENTS OF THE FRUIT FIBERS OF TRICHOSANTHES CUCUMERINA

Matee Buaprrom[1], Sunanta Wangkarn[2], Anon Chindaduang[1] and Apichart Suksamrarn[1,*]
[1] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand;
[2] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand;
e-mail address: apichart@ram1.ru.ac.th

Abstract: Investigation of the fruit fibers of Trichosanthes cucumerina resulted in the isolation of five triterpenes: cucurbitacin B (1), cucurbitacin E (2), isocucurbitacin B (3), 23,24-dihydroisocucurbitacin B (4) and 23,24-dihydrocucurbitacin E (5). The sterols β-sitosterol and stigmasterol were also isolated. Structures of these compounds were identified based on spectroscopic evidence.

C3_C0252 Chemical Constituents and Biological Activities of Erythrina stricta

Thitima Rukachaisirikul, Phongsak Innok, Amporn Saekee, Chatchana Tharibun, Sudarut Watkuolham and Apichart Suksamran
Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand
e-mail address: thitima@ram1.ru.ac.th

Abstract: Investigation of the roots of Erythrina stricta afforded twelve compounds: alkyl trans-ferulate (**1**), a mixture of β-sitosterol (**2**) and stigmasterol (**3**), erystagallin A (**4**), erythrabissin-1 (**5**), sandwicensin (**6**), erythrabyssin II (**7**), 5-hydroxysophoranone (**8**), sophoradiol (**9**), soyasapogenol B (**10**), 8-oxoerythrinine (**11**) and erythratine (**12**). Their structures were identified by spectroscopic methods. The isolated compounds were tested for antiplasmodial activity, antimycobacterial activity and cytotoxicity.

C3_C0254 Chemical Constituents of the Bark of *Dalbergia glomeriflora*

Thitima Rukachaisirikul, Siriyaporn Thaleongwuttiwong, Charoenchai Jaisawang, Thussanee Chunet, Phunticha Phunpai and Apichart Suksamran
Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand
e-mail address: thitima@ram1.ru.ac.th

Abstract: Investigation of the bark of *Dalbergia glomeriflora* resulted in the isolation of eleven compounds: lupenone (1), lupeol acetate (2), lupeol (3), a mixture of β-sitosterol (4) and stigmasterol (5), biochanin A (6), vestitol (7), (+)-medicarpin (8), formononetin (9), texasin (10) and 8-C-glycosyl-7-methoxy-4',5-dihydroxyisoflavone (11). Their structures were identified by spectroscopic methods.

C3_C0255 BIOTRANSFORMATION OF SOME SEX HORMONES BY *BACILLUS MEGATERIUM* NRRL B-938

Somkiat Kongkun[1], Oratai Sukcharoen[2], Boon-ek Yingyongnarongkul[1] and Apichart Suksamrarn[1,*]
[1] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand;
e-mail address: apichart@ram1.ru.ac.th
[2] Department of Biotechnology, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand.

Abstract: 4-Androsten-3,17-dione (1) underwent allylic hydroxylation to 6β-hydroxy-4-androsten-3,17-dione (2) by the bacterial *Bacillus megaterium* NRRL B-938. *trans*-Dehydroandrosterone (3) was similarly biotransformed into the corresponding 7α-hydroxy analogue whereas 17α-hydroxyprogesterone (5) was converted to 17α,20-dihydroxy-4-pregnen-3-one (6) and

6β,17α,20-trihydroxy-4-pregnen-3-one (7).

C4_C0002 THE CONFINEMENT EFFECT ON ADSORPTION OF METHANE, PROPANE AND BENZENE ON THE FE-ZSM-5 ZEOLITE: ONIOM METHOD

Suwat Pabchanda
Department of Chemistry, Faculty of Science, Ubon Rajathanee University, Ubon Ratchathani 34190, Thailand.
E-mail: pabchanda@gmail.com, Fax: 0-4543-3113

Abstract: We have employed ONIOM2(B3LYP/6-311+G(3df,2p):UFF) to investigate the adsorption of methane, propane and benzene on the Fe-ZSM-5 zeolite, prior to its selective oxidation of methane to methanol, propane to propene and benzene to phenol, respectively. The adsorption energies of CH_4/Fe-ZSM-5, C_3H_8/Fe-ZSM-5 and C_6H_6/Fe-ZSM-5 complexes are evaluated to be -6.1, -13.5 and -23.2 kcal/mol, respectively. The results demonstrate that the adsorption properties of hydrocarbon compounds on the Fe-ZSM-5 depend not only on the specific environment of zeolite, but also on the molecular size of adsorbate.

C4_C0007 DFT INVESTIGATION OF STRUCTURES OF NITROSAMINE ISOMERS AND THEIR TRANSFORMATIONS IN GAS PHASE

Banchob Wanno, Vithaya Ruangpornvisuti
Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

Abstract: The geometrical structures of H_2NNO nitrosamine isomers have been obtained by geometry optimizations using the DFT method at the RB3LYP/aug-cc-pVDZ level of theory. One amino, 4 imino tautomers, 2 zwitterionic and 2 oxadiaziridine isomers of the H_2NNO nitrosamine have been found. The most stable species of the nitrosamine isomers existing as an amino form has been found. Energetics, thermodynamic properties, rate constants and equilibrium constants of all transformation reactions have been determined. The energy profile for the transformation reactions of the nitrosamine isomers has been presented.

C4_C0015 Formation of Nanoribbons of Polyfluorene and Poly(fluorene-co-anthracene) on Solid Substrates

Parinda Manorut[1], Nipaphat Charoenthai[1], Rakchart Traiphol[1*], Toemsak Srikhirin[2], Teerakiat Kerdcharoen[2], Tanakorn Osotchan[2]
[1] Department of Chemistry, Faculty of Science, Naresuan University, Phitsanulok 65000, Thailand and [2]Department of Physics, Faculty of Science, Mahidol University and Center of Nanoscience and Nanotechnology, Faculty of Science, Mahidol University, Rama 6 Road, Ratchathewi, Bangkok 10400, Thailand
* Corresponding author e-mail: rakchartt@nu.ac.th

Abstract: An ability to construct nanoscale structures of conducting polymers is a crucial step for the development of future nanoelectronics. In this study, growth of nanoscale ribbons of polyfluorene (PF) and random poly(fluorene-co-anthracene) (PF-co-Ant) on solid substrates is investigated by utilizing atomic force microscopy (AFM). By self-assembling the 0.3 and 0.05 mg/mL PF solutions onto a silicon wafer, the interconnected fibrils of nanoribbons are obtained. Similar structure is detected in thin films of copolymers PF-co-Ant. However, cross section diameter of the nanoribbons varies with ratio of anthracene unit in backbone. In addition, increasing mole ratio of anthracence unit to 20% is found to retard to formation of nanoribbons. Decreasing polymer concentration to 0.01 mg/mL causes the formation of polymer droplets. Using the mica substrate is also not favorable for the formation of nanoribbons.

C4_C0016 Physical Gelation of Conjugated Polymer in Dilute Solutions: Solvent Effects

Pawanrat Moltat[1], Nattapong Nujaikong[1], Rakchart Traiphol[1*], Toemsak Srikhirin[2]
[1] Department of Chemistry, Faculty of Science, Naresuan University, Phitsanulok 65000, Thailand and [2]Department of Physics, Faculty of Science, Mahidol University and Center of Nanoscience and Nanotechnology, Faculty of Science, Mahidol University, Rama 6 Road, Ratchathewi, Bangkok 10400, Thailand
* Corresponding author e-mail: rakchartt@nu.ac.th

Abstract: Conjugated polymers dispersed in solutions can exhibit various phases such as physical gel and liquid crystal. In this study, we have found that solution of poly[2-methoxy, 5-(2'-ethylhexoxy)-*p*-phenylene vinylene] (MEH-PPV) in toluene forms room temperature gel phase at relatively low concentration, 20 mg/mL. The gelation is characterized by mean of viscosity change. Increasing temperature causes the gel to transform into solution phase. Fluorescence spectroscopy and nuclear magnetic resonance spectroscopy (NMR) are utilized to determine gel-sol transition temperature. The study by differential scanning calorimetry (DSC) indicates that the gel is a disorder phase. The gelation of MEH-PPV is found to be solvent selective. Dissolving same concentration of the polymer in tetrahydrofuran, chloroform and pyridine does not lead to gelation. The NMR study indicates strong π-π interaction between conjugated backbone and toluene, which is probably a major reason responsible the gelation.

C4_C0017 Copolymerization Approach for Reducing Aggregation of Blue-Light-Emitting Polyfluorene

Sriwipa Puyati, Nanthawan Sangthong, Nipaphat Charoenthai, Rakchart Traiphol*,
Department of Chemistry, Faculty of Science, Naresuan University, Phitsanulok 65000, Thailand

*Corresponding author e-mail: rakchartt@nu.ac.th

Abstract: Our research investigates the aggregation in solutions of polyfluorene-based copolymers by utilizing uv-visible absorption and steady state fluorescence spectroscopy. Isolated chains of polyfluorene dispersed in good solvent toluene are driven to aggregate by addition of poor solvent, methanol. The polymer aggregation allows electronic interactions between conjugated chains resulting in the novel electronic species distinct from the isolated chains. The existence of the aggregates is characterized by the detection of red-shift peak in the absorption and emission spectra. Quantity of the aggregates relative to the isolated chains is slightly affected as 5, 10 and 15 mol% of the "anthracene defect" is randomly introduced into the polyfluorene backbone, compared to system of homopolymer polyfluorene. Further increasing the anthracence mole ratio to 20%, however, causes the aggregation to significantly diminish in the same condition. The presence of anthracene in the copolymers also systematically affects the electronic properties of isolated chains.

C4_C0020 Role of Chain Conformation on Aggregation Efficiency of Conjugated Polymer in Solution

Nipaphat Charoenthai, Rakchart Traiphol
Department of Chemistry, Faculty of Science, Naresuan University, Phitsanulok 65000, Thailand *Corresponding author e-mail: rakchartt@nu.ac.th

Abstract: This research investigates the aggregation behavior of poly[2-methoxy, 5-(2'-ethylhexoxy)-*p*-phenylene vinylene] (MEH-PPV) in various solvents with different structures and polarity by using UV/vis absorption and emission spectroscopy. The aggregation of conjugated polymers is induced by adding a poor solvent into a solution of MEH-PPV in good solvents. The aggregation is indicated by the appearance of distinct red-shift peak in absorption and emission spectra. In each system, the aggregation is found to take place when about 80 %v/v of cyclohexane is added. The aggregation appears to occur easier in the system of mixed aromatic solvents and cyclohexane. In the system of pyridine and cyclohexane, however, only a small amount of aggregates is detected. We propose that the efficiency of the aggregation depends on the magnitude of the extension or collapse of isolated chains dissolved in various solvents with different structures and polarity. The strong coupling between MEH-PPV backbone and the aromatic solvents are explored as well. This could be another factor affecting the aggregation efficiency.

C4_C0021 Change of Chain Conformation Induces Multiple Photo-emissions from Conjugated Polymer

Rakchart Traiphol
Department of Chemistry, Faculty of Science, Naresuan University, Phitsanulok 65000, Thailand
Corresponding author e-mail: rakchartt@nu.ac.th

Abstract: Conjugated polymer can be considered as a chain constituting of multiple chromophores with various conjugation lengths. These chromophores are connected together via physical or chemical defects. Due to efficient intrachain energy transfer the photo-emission of conjugated chains normally takes place from the chromophores with longest conjugation length. In this study, we have found that various chromophores of poly[2-methoxy, 5-(2'-ethylhexoxy)-*p*-phenylene vinylene] (MEH-PPV) dissolved in poor solvents can emit photons simultaneously. The unfavorable polymer-solvent interactions in this system induce the individual conjugated chains to collapse and aggregate. The increase of intrachain disorder suppresses the energy transfer process, allowing the emissions from chromophores with various conjugation lengths to occur. The emission from aggregates is also detected. These types of photo-emissions depend on various factors such as polymer concentration, temperature and excitation wavelength.

C4_C0026 HYDROXIDE, PROTON AND WATER ADSORPTIONS ON CLOSED SINGLE-WALLED CARBON NANOTUBES

Raina Wanbayor, Vithaya Ruangpornvisuti
Supramolecular Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

Abstract: The adsorptions of hydroxide, proton and water on the closed armchair (5,5) single-walled carbon nanotube (SWCNT) of sizes $C40+C20_n$, n = 2 and 3 were studied using Hartree-Fock and two-layered ONIOM(MO:MO). Based on the HF/3-21G computations, the reaction energies between the SWCNT of size C40+C40 and proton, and hydroxide, computed are -224.71 and -144.77 kcal/mol, respectively and the reaction energy with hydroxide ion of the protonated SWCNT are -221.13 kcal/mol. The interaction energies of the protonated, hydroxylated and zwitterionic-water added SWCNTs with a water molecule are -14.05, -13.65 and -14.97 kcal/mol, respectively.

C4_C0027 ON THE LOWER SUSCEPTIBILITY OF OSELTAMIVIR TO AVIAN INFLUENZA NEURAMINIDASE SUBTYPE N1 THAN TO N2 AND N9.

Ornjira Aruksakunwong, Maturos Malaisree, Panita Decha, Pornthep Sompornpisut, Vudhichai Parasuk, Somsak Pianwanit, Supot Hannongbua
Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok , Thailand.
Email:upot@atc.atccu.chula.ac.th

Abstract: Since its first emergence in Hong Kong in 1997, the influenza A (H5N1) infections have caused many human deaths. Oseltamivir (OTV), which is known to against a broad range of influenza viruses, was found to be less effective for

neuraminidase subtype N1 in comparison to N2 and N9. Molecular dynamics simulations were carried out for the three complexes, OTV-N1, OTV-N2 and OTV-N9. Dramatic changes were observed on the OTV conformation in which two bulky side chains, $-NHCOCH_3$ and $-OC_5H_{11}$, were rotated in order to adjust its size to fit into the N1 catalytic site. This change leads directly to the rearrangements of the OTV's environment. The calculated ligand/enzyme binding free energies of -7.20, -13.44 and -13.29 kcal/mol agree totally with their inhibitory activities in term of the experimental *IC50* of 36.1 - 53.2 nM, 1.9 - 2.7 nM and 9.5 - 17.7 nM for the OTV-N1, OTV-N2 and OTV-N9 complexes, respectively.

C4_C0028 ADSORPTION OF SODIUM DODECYL SULFATE ON SILICA PARTICLES MODIFIED BY POLYETHYLENEIMINE

Sorapong Janhom[1*], Romran Chusie[2]
[1] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand.
[2] Science Department, Faculty of Science and Technology, Prince of Songkla University, Pattani Campus, Pattani, Thailand.

Abstract: Silica particles were modified by polyethyleneimine (PEI) in order to produce the particles that readily adsorbed sodium dodecyl sulfate (SDS) molecules. The adsorption of PEI on silica particles was studied and the adsorption isotherm obtained was identified to be a Langmuir type. The adsorption of SDS on PEI-silica particles was then investigated and the results showed that the adsorbed amount of SDS increase with increasing in SDS concentration. The influence of NaCl on SDS adsorption on the PEI-silica particles was also studied. It was revealed that increasing in NaCl concentration decreased the absorbed amount of SDS on PEI-silica particles. In addition, the SDS adsorption on PEI-silica particles at various pH indicated that the adsorbed amount of SDS increased following the decreasing in pH. This result might be caused by protonation at low pH of amine group in PEI chain which readily interact with negative charge of sulfate ion of SDS molecules.

C4_C0034 MOLECULAR SIMULATION STUDIES OF THE STRUCTURE, INTERACTION AND DIFFUSION OF DRUG IN CHITOSAN MATRIX

Natthida Ragkapao, Visit Vao-soongnern*
School of Chemistry and Laboratory of Computational and Applied Polymer Science (LCAPS), Institute of Science, Suranaree University of Technology, Nakhon Ratchasima, Thailand.
E-mail: visit@sut.ac.th, Fax: 04-4224-185

Abstract: Molecular modeling has been performed at atomistic level of chitosan and its complex with aspirin i.e. a model of drug control-release system. Deacetylation of chitin acetylamine groups by chemical reaction has a significant effect on the conformational properties of the glycosidic bonds linking two repeat units. Both the location and the relative energies of the low energy areas of the potential energy surfaces slightly differ. The amorphous bulk model was then constructed to model the solid state of these polysaccharides. The results reported, including energetics, chain dimention, torsional distribution, pair distribution function and X-Ray structure factor, provide a detailed description of the disordered state of the polysaccharide chains as well as an interaction with a model drug. The amine groups in chitosan were found to interact strongly with the carbonyl groups in Aspirin. This interaction, however, existed only when the amine groups was in its protonated form. The diffusion coefficient of a drug model in chitosan matrix was also calculated.

C4_C0035 ATOMISTIC MOLECULAR MODELING ON POLYMER BLEND MISCIBILITY: POLYETHYLENE OXIDE/ POLYETHYLENE IMINE SYSTEM

Jittima Chaodamrongsakul[1,2], Supagorn Rugmai[3,4], Wantana Klysubun[4], Visit Vao-soongnern[1,2*]
Laboratory of Computational and Applied Polymer Science (LCAPS)[1], School of Chemistry[2] and School of Physics[3], Institute of Science, Suranaree University of Technology, National Synchroton Research Center[4], Nakhon Ratchasima, Thailand.
E-mail: visit@sut.ac.th, Fax: 04-4224-185

Abstract: Computer simulations play an important role in designing new polymers as well as in predicting properties of existing polymers. In this work, the blend compatibility of poly(ethylene oxide), PEO, $(\text{--}CH_2CH_2O\text{--})_n$ with poly(ethylene imine), PEI, $(\text{--}CH_2CH_2NH\text{--})_n$,a blend model of the polymer host for solid electrolytes system, was studied over the wide range of compositions. By means of fully atomistic molecular simulation the solubility parameters for pure PEO and PEI were calculated and the results were in good agreement with the literature values. These two simulated solubility parameters were similar indicating that the PEO/PEI blend system was miscible. Also, the Flory-Huggins interaction parameter (□) of the blends computed using the atomistic simulation confirmed the blend compatibility for all compositions containing PEI.

C4_C0039 Adsorption Isotherm of Cu^{2+} by chitosan form shrimps and crabs shells

Dr.Sudaporn Tangkawanit, Thanyapat Thiantongin, Siriwan Kaewdee, Ampaporn Prompradit
Department of Chemistry, Faculty of science, Ubon Ratchathani Rajabhat University, Ubon Ratchathani 34000, Thailand
Email address: tangkawa@yahoo.com, poo_cheme@yahoo.com

Abstract: This work studied on adsorption isotherm of Cu^{2+} by Chitosan from shrimps and crabs shells. Degree of deacetylation (%DD) of standard chitosan, chitosan from shrimps and crabs shells were determined by FT-IR spectroscopy of 83.07, 80.26 and 78.94 %, respectively and titration technique of 82.20, 80.38 and 78.25 %, respectively. The molecular weight of standard chitosan, chitosan from shrimps and crabs shells were found to be $1.07x10^6$, $8.27x10^5$ and $7.43x10^5$ g/mol, respectively. Adsorption isotherms of Cu^{2+} in standard chitosan, chitosan from shrimps and crabs shells could be well fitted by the Langmuir equation with the constants K_L were 24.62, 17.26 and 16.57 mg/g; b were 0.0060, 0.0064 and 0.0046

L/mg, respectively. It can be concluded that chitosan from shrimps and crabs shells are effective adsorbents for the Cu^{2+}.

C4_C0065 Characterization of γ-oryzanol encapsulated in Solid lipid nanopaticles for drug delivery

Surachai Limpakdee[1], Uracha Ruktanonchai[2], Siwaporn Meejoo[1]

[1] School of Chemistry, Faculty of Science, Mahidol University, Rama VI road, Bangkok, 10400
E-mail:scsmj@mahidol.ac.th, Tel:02-201-5164, Fax: 02-354-7151

[2] National Nanotechnology Center, National Science and Technology Development Agency, 111 Thailand Science Park, Paholyothing Rd., Klong 1, Klong Luang, Pathumthani 12120

Abstract: Aqueous dispersions of solid lipid nanoparticles (SLN) are currently promising drug carrier system, especially for dermal application. This research has focused on the production of cetyl-palmitate nanoparticles encapsulated with γ-oryzanol, an anti-oxidant compound found in rice bran oil extract. The nanoparticles were produced by hot homogenization method from 10% cetyl-palmitate and 2.5% pluronic F68 in water. Loading of γ-oryzanol were varied between 0.0 to 5.0 %w/w. Structures of the nanoparticles are confirmed by using powder x-ray diffraction, and physical stability of nanoparticles at 0, 30, 60 days were examined by measuring of their hydrodynamic diameters, zeta potentials using photon correlation spectroscopy and by evaluating of melting enthalpy and recrystallization indices using differential scanning calorimetry. Our results demonstrate that hydrodynamic diameters of SLN were in the 220 to 280 nm range and zeta potential between –27 to –35 mV. The SLN loaded with 1.5% oryzanol have the highest stability as their physical and thermodynamic properties are slightly different from the freshly prepared nanoparticles.

C4_C0074 Molecular Dynamic Simulations of M2 Channel: Structural properties and Ionization State Dependence of Selectivity Filter Residues in Proton Transport Process

Chittima Laohpongspaisan, Pornthep Sompornpisut, Supot Hannongbua
Department of Chemistry, Faculty of Science, Chulalongkorn University, Patumwan, Bangkok, 10330 Thailand.

Abstract: Molecular dynamics (MD) simulation of M2 channel have been performed to examine the ionization state dependence of selectivity filter residues in the proton transport process. Five different protonation states (PS) of M2 histidine which are non-PS (0H-M2), single PS (1H-M2), double PS at adjacent position (2aH-M2), double PS at diagonal position (2dH-M2), and quadruple PS (4H-M2) were embedded in a solvent system containing water and lipid bilayer, 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC). MD simulation were carried out for 8 ns at different protonation states, the selectivity filter residue of M2 channel. The results shown that water molecule cannot move through the constrictive region of the channel in non-protonated state. This corresponds to the closed state of the M2 channel. The channel is partially open for the 1H-M2, 2aH-M2, 2dH-M2, and fully open for 4H-M2 PS system.

C4_C0082 Physical and Mechanical Properties Improvement of Fibroin Membrane from Silk Waste by Low Molecular Weight Polyethylene Glycol Diglycidyl Ether

Piyarut Moonsri [1], Ruangsri Watanesk[1], Surasak Watanesk[1], Hataichanok Neimsup[1], Richard L. Deming[2].

[1] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.
E-mail Address; piyarutto@hotmail.com

[2] Department of Chemistry and Biochemistry, California State University , Fullerton, CA 92831, U.S.A.

Abstract: Modification of fibroin from silk waste, Bombyx mori, was carried out by adding the crosslinking agent, polyethylene glycol diglycidyl ether (PEGDE, MW 526), into fibroin solution. Then the mixture solution was left on polystyrene dish at 60 °C for 9 hrs until membrane formation occured. The membrane surface, investigated by Scanning Electron Microscopy, exhibited the influence of crosslinker on membrane porosity. The secondary structure of the membranes, characterized by Fourier Transform Infrared Spectroscopy, showed the transformation of the modified fibroin membrane from random coil to β-sheet. Results from UV–visible spectrophotometry showed that the modified fibroin membranes had high water resistance within the pH range of 4-10. In addition, the crosslinker could remarkably improved the compliance and tenacity of the membrane. These features are expected to be useful in biosensing applications.

C4_C0093 Copper(I) Iodide Complex with Triphenylphosphine and Phenylthiourea

Ruthairat Nimthong[1], Chaveng Pakawatchai[1], Yupa Thunyasirikul[1] and Saowanit Saithong[1]

[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hatyai, Songkhla, 90112 Thailand.
e-mail address: opela_c@hotmail.com

Abstract: The complex of bis(triphenylphosphine)(phenylthiourea)iodocopper(I), $[Cu(PPh_3)_2(ptu)I]$ was prepared by the reaction of copper(I) iodide with phenylthiourea(ptu) and triphenylphosphine (PPh_3) in suitable condition. The crystal structure has been determined by single crystal X-ray diffraction method. The complex crystallizes in triclinic system space group P_1 with cell parameters a = 10.9505(9), b = 18.7294(15), c = 21.3731(18) Å, α = 67.4220(10), β = 77.2150(10), γ = 73.2240(10)°, R = 0.0503. The complex is monomeric with the copper atom is distorted tetrahedrally coordinated by two PPh_3 molecules, one ptu molecules and one iodine atom.

C4-C0096 A THEORETICAL INVESTIGATION ON STRUCTURAL AND ENERGETIC PROPERTIES OF ALUMINIUM SUBSTITUTION, PROTON AND CATIONS ADSORPTION IN A NATURAL ZEOLITE-CLINOPTILOLITE

Chan Inntam[1], Pornpan Pungpo[1] and Nikorn Seangsuwan[1]

[1] Research Unit of Computational Chemistry (RUCC), Chemistry Department, Faculty of Science, Ubon Rajathanee University, Warinchamrap, Ubon Ratchathani; THAILAND
E-mail: ichan@sci.ubu.ac.th, Fax: (66)45288379

Abstract: Structural and energetic properties of proton and cations adsorption in Clinoptilolite (HEU) have been studied by means of Density Functional Theory (DFT) using B3LYP/6-31G* level of calculation. To elucidate such properties occurring in the HEU framework, a 14T cluster model is employed to represent the framework. The results emphasize on the framework Al distribution and the location of extra-framework cations. Al is predicted to be preferentially localized at the T1 and T2 crystallographic sites. The substitution at other sites requests the energy in order of 60 kJ mol^{-1}. For proton adsorption, the proton prefers to adsorb at the O atom connected to the substituted Al atom. The most stable adsorption complex relates to the 97 pm of O–H distance and 129° of Al–O–Si angle. The corresponding proton affinity is calculated to be 1313 kJ mol^{-1}.

C4_C0099 CONFORMATIONAL ANALYSIS OF CYCLOHEPTAPEPTIDE BY NMR AND STOCHASTIC DYNAMIC SIMULATION

Sarote Boonseng, Ekasith Somsook, Vichai Reutrakul
Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok, Thailand.

Abstract: The cycloheptapeptide consisting of seven amino acids [Ala(β-OAc)(β-Fur3)-Ile-MeAla-Ala(β-OAc)(β-Fur3)-Ile-Sar(α-2,3-Me_2cyclopropanyl)] was investigated. Three-dimensional structures of cycloheptapeptide were determined in solution by NMR and Stochastic dynamics simulations. The stereochemistry of all α-carbon and β-carbon of isoleucine residues are assumed to be the identical as natural amino acids. Eight isomers (RRC, RRC2, RSC, RSC2, SRC, SRC2, SSC and SSC2) of cycloheptapeptide were selected for this study by varying the stereochemistry at C_γ of Ala(β-Oac)(β-Fur3) residues and the configurations of the cis-form (C-up, C2-down) at Sar(α-2,3-Me_2cyclopropanyl) residue. NMR spectra of cycloheptapeptide were collected in $CDCl_3$ at ambient temperature. The resonance assignments were carried out using 1D and 2D-NMR. Distance (calculated from the inverse of the sixth power of distances) and torsional angle restraints (calculated from Karplus equations) were used as the input data for the restrained simulated with AMBER force field using Stochastic dynamics simulations in implicit solvents ($CHCl_3$) at 300 K for 10 ns. The final energies from each method for each possible isomer were compared to provide that the SRC isomer had the lowest energy.

C4_C0106 A SYSTEMATIC FIRST-PRINCIPLES STUDY OF THE STRUCTURE AND FUNCTION OF BI-FUNCTIONAL ZEOLITE CATALYSTS

Siriporn Jungsuttiwong and Jarun Lomratsiri
Research Unit of Computational Chemistry (RUCC), Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani, Thailand, 34190
E-mail: jsiripor@sci.ubu.ac.th, Fax: (66-45)288379

Abstract: A systematic first-principles study of the structure of Pt-H-ZSM-5, bi-functional zeolite catalysts, have been carry out by a new E-ONIOM approach which is improved to represent the long-range Madelung potential from the extended zeolite framework. Using the hybrid B3LYP density functional theory, we found that the preferable structure of Pt-H-ZSM-5 complex is forming 5-member ring-like structure by the Pt atom interacts with acidic proton and the oxygen adjacent to Al atom in the zeolite framework. The binding energy of Pt on the Brønsted acid was calculated to be 35.45 kcal/mol. The calculated Pt-O1 (Pt atom and Brønsted oxygen) and Pt-O2 (Pt atom and the nearest bridging oxygen) distances are 2.86 and 2.09 Å respectively, this results agree very well with the experimental observation. The adsorption energies obtained by E-ONIOM is significantly different from the value obtained from the cluster model. This indicates that the effects of Madelung potential due to atoms outside the quantum cluster by using our E-ONIOM method are definitely crucial.

C4_C0109 CONFORMATIONAL ANALYSIS OF MELEZITOSE BY NMR AND MOLECULAR DYNAMICS SIMULATIONS

Ekasith Somsook and Wiwaporn Soodsawang
Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd. Rachathewi, Bangkok, 10400, Thailand.

Abstract: The structure of O-α-D-glucopyranosyl-(1→2)-O-β-D-fructofuranosyl-(3→1)-α-D-glucopyranoside or melezitose, a trisaccharide, was investigated in solution by NMR and molecular dynamics (MD) simulations. NMR spectra of melezitose were collected in D_2O at ambient temperature on a Bruker DRX-500 spectrometer. The chemical shift assignments were determined by 1D-^{1}H, 1D-^{13}C, 1D-^{13}C-DEPT, 2D-^{1}H-DQF-COSY, 2D-^{1}H-^{13}C-HMQC and 2D-^{1}H-^{13}C-HMBC experiments. 2D-^{1}H-NOESY experiments were collected at 0.30 s, 0.45 s, 0.60 s, 0.75 s, and 1.00 s. The distance restraints between proton pairs were calculated by using the average distance between H_1 and H_2 of both glucose units and the torsion angle restraints of the glycosidic bonds were calculated from a Karplus equation. Atomic coordinates of melezitose structure was generated using Macromodel v8.1. The topology and coordinate files were generated for minimization, simulated annealing, and dynamics simulations of melezitose with restraints and unrestraints, both in vacuo and including explicit solvent using the SANDER module of AMBER. The major and minor conformations were observed from the MD trajectories.

C4_C0121 SYNTHESIS OF ZEOLITE FROM BOTTOM ASH AND FLY ASH.

Naruemon Setthaya*, Kedsarin Pimraksa
Department of Industrial Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand .
E-mail address: naruemon_se@hotmail.com

Abstract: Suitable conditions for zeolite synthesis using hydrothermal process were studied. Used raw materials compose of coal combustion by-products ; bottom ash and fly ash. Factors effecting to the zeolite synthesis are types and concentrations of alkaline solution. The synthesized zeolite will be analysed the quality and quantity. It was found that, using bottom ash with 5M of potassium hydroxide solution at 100°C for 24 h under the ambient atmosphere provided zeolite type named as Phillipsite-K and potassium aluminum silicate hydrate. While using fly ash under the same conditions of the synthesis provided only potassium aluminum silicate hydrate. Using fly ash with 3M of sodium hydroxide solution at 100°C for 24 h under the ambient atmosphere provided zeolite type named as sodalite. While using bottom ash under the same conditions of the synthesis provided sodium magnesium chloride silicate hydroxide. The synthesis percent yields were in a range of 95-98.

C4_C0150 PREPARATION OF ELECTRICAL CONDUCTIVE ABS COMPOSITE FOR BIPOLAR PLATES IN PEM FUEL CELL

Somruthai Tunma, Jantrawan Pumchusak
Department of Industrial Chemistry, Faculty of Science, Chiang Mai University, T.Suthep, A.Muang , Chiang Mai, Thailand.
E-mail:stunma@hotmail.com, jantra.t@chiangmai.ac.th

Abstract: Today, the development of PEM fuel cell is active for the versatile application. Bipolar plate (BP) is a key component of PEM fuel cell when series of fuel cell are stacked in order to increase the voltage of fuel cell. BP conducts electrical current from cell to cell. Furthermore, BP is the major part which indicates volume, weight and cost of PEM fuel cell stacks. Therefore, low cost materials are searched . ABS composite was studied in this research. Graphite, carbon black and carbon fiber were used as electrical conductive fillers. The effect of content and composition of fillers and the incorporation of fillers including the length of carbon fiber on the electrical properties of polymer composite were studied.

C4_C0152 THE DIELECTRIC PROPERTIES OF BARIUM ZIRCONATE TITANATE CERAMICS PREPARED BY AUTO-COMBUSTION METHOD.

Pornsatit Sookchoo*, Laddawan Pdungsap
Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Rd., Bangkok, 10400, Thailand.
E-mail:toy_another@yahoo.com

Abstract: $Ba(Zr_yTi_{1-y})O_3$ (y = 0.15, 0.20) ceramics were prepared by auto-combustion method. The structure and electrical properties have been investigated. The XRD patterns of prepared BZT ceramics show quite pure perovskite phase. The dielectric constant of $Ba(Zr_{0.15}Ti_{0.85})O_3$ and $Ba(Zr_{0.20}Ti_{0.80})O_3$ was about 2000 and 3500, respectively.

C4_C0156 ANALYSIS OF SURFACE CONTAMINATION BY ATR FT-IR MICROSPECTROSCOPY

Narumon Pattayagorn[1], Sanong Ekgasit [2], Pol. Col. Thada Tangsrisuk[3]
[1] Program in Petrochemistry and Polymer Science, Faculty of science, Chulalongkorn University, Bangkok, Thailand.
E-mail: cherry_toad@hotmail.com
[2] Sensor Research Unit, Department of Chemistry, Faculty of science, Chulalongkorn University, Bangkok, Thailand.
E-mail: sanong.e@chula.ac.th
[3] Central Institute of Forensic Science Thailand, Bangkok 10880, Thailand.

Abstract: The dome shape Ge μIRE is developed for ATR FT-IR spectral acquisition using an infrared microscope. The ATR spectrum under total internal reflection phenomenon within the germanium IRE can be collected. Due to the small sampling area of the Ge tip, a small sample can be analyzed by the novel Ge μIRE. The objective of the research is to develop ATR FT-IR technique for analysis of surface contamination. Contamination on a surface can be deposited on Ge μIRE by pressing the mineral oil coated IRE on the surface. This novel sampling method is called the *"contact and collect"* technique. This technique is non-destructive, does not require additional sample preparation and take shot time of analysis.

C4_C0157 FORENSIC ANALYSIS OF AUTOMOTIVE PAINTS BY ATR FT-IR MICROSPECTROSCOPY

Pornpan Watcharasanyakorn[1], Sanong Ekasit[2]
[1] Program in Petrochemical and Polymer science, Faculty of science, Chulalongkorn University, Bangkok,10330, Thailand.
E-mail: nu_nannaja@yahoo.com, Tel: (662)218-7585
[2] Sensor Research Unit, Department of chemistry, Faculty of science, Chulalongkorn University, Bangkok,10330, Thailand.
E-mail: Sanong.e@chula.ac.th, Tel: (662)218-7585

Abstract: The examination of automotive paints is important in an accident investigation. In this work, the characteristic of automotive paints observed by ATR FT-IR microspectroscopy were studied. The technique has short analysis time and non-destructive. The novel diamond μIRE with a gem quality round brilliant cut natural diamond and the Ge μIRE with a dome shape Ge was employed for spectral acquisition using an infrared microscope. The small paint fragment can be studied diamond μIRE and Ge μIRE since both IREs have small sampling area. The spectra acquired by diamond μIRE and Ge μIRE were the same as those acquired by conventional ATR. The spectra from different paints show different spectral features due

to different compositions such as binder, pigment, and additive. The chemical information of automotive paint can be acquired while the information can be applied for forensic analysis.

C4_C0159 FORENSIC ANALYSIS OF LIPSTICKS BY ATR FT-IR MICROSPECTROSCOPY

Prapimpan Supmuang[1], Sanong Ekgasit[2]
[1] Program of Petrochemistry and Polymer science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.
E-mail: nan_attja@yahoo.co.th, Tel: (622)218-7585
[2] Sensor Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.
E-mail: Sanong.e@chula .ac.th, Tel: (622)218-7585

Abstract: The diamond μIRE with a gem quality faceted diamond as an internal reflection element (IRE) and Ge μIRE for ATR FT-IR spectral acquisition with an infrared microscope were employed for forensic analysis. This technique does not require an additional sample preparation and has short analysis time. Due to the small sampling area of the diamond μIRE and Ge μIRE, the small sample can be employed by the analysis. In this work, forensic analysis of lipsticks by diamond μIRE and Ge μIRE were demonstrated. Minute smears of lipstick can be analyzed while the chemical information of lipsticks on various substrates were achieved without any interference from the glass, tissue paper substrate. The spectra acquired by diamond μIRE and Ge μIRE were in good agreement to those acquired by the conventional ATR technique.

C4_C0160 PERTURBATION OF METHANOL IN THE BELOUSOV-ZHABOTINSKY REACTION: EXPERIMENTAL AND CALCULATED SHAPE OF OSCILLATIONS

Siriwat Sansuk[1], Atchara Sirimungkala[1], Somkiat Srijaranai[1], and Tawun Remsungnen[2]
[1] Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen, Thailand.
E-mail:siriwatsansuk4@hotmail.com
[2] Department of Mathematics, Faculty of Science, Khon Kaen University, Khon Kaen, Thailand.

Abstract: To follow the perturbation of methanol, some selected conditions of the Belousov–Zhabotinsky (BZ) reaction were used. Results show that the induction period and the frequency of the oscillations increase whereas the amplitude of the oscillations decreases. Kinetics of the bromate-methanol reaction was investigated. In the case of excess bromate, we treated the experimental curves according to a pseudo-first order kinetics. The rate constant of the bromate-methanol reaction, 5.31×10^{-3} $M^{-1}s^{-1}$, was obtained. The model of the bromate-methanol reaction was simulated by adjusting the rate constant to 8.5×10^{-4} $M^{-1}s^{-1}$. By inserting the perturbating reaction into the MBM model, the calculations are in good qualitative agreement with the experiments.

C4_C0161 HOMOGENEITY OF POLYMER COMPOSITES INVESTIGATED BY ATR FT-IR MICROSPECTROSCOPY

Duangta Tongsakul[1], Chuchaat Thammacharoen[2], Sanong Ekgasit[2]
[1] Program in Petrochemistry and Polymer science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.
Email: duangta_t@hotmail.com, Tel: (662)218-7585
[2] Sensor Research Unit, Department of chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.
Email: Sanong.e@chula.ac.th

Abtract: For polymer composites, the effective dispersion of filler within the polymer matrix in combination with interfacial adhesion, filler, and polymer can substantially improve mechanical properties of the composites. In this study, homogeneity of polymer composites were investigated by ATR FT-IR microspctroscopy by using diamond μIRE. Due to its inherent hardness and sharp tip, the diamond μIRE can be employed for probing depth dependent properties of polymer composites. The uniform dispersion of filler throughout the polymer matrix shows the same absorbption magnitudes and at various depth. As the absorption is directly related to concentration, the diamond μIRE can be employed for the determination of homogeneity of composites. This technique does not require additional sample preparation, it has short analysis of time while chemical information can be obtained.

C4_C0162 FORENSIC ANALYSIS OF HUMAN HAIR BY ATR FT-IR MICROSPECTROSCOPY

Suwimol Naranitad[1], Sanong Ekasit[2], Chuchaat Thammacharoen[2]
[1] Program of Petrochemistry and Polymer science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.
E-mail:gad_47_1@hotmail.com, Tel: (622)218-7585
[2] Sensor Research unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.
E-mail: Sanong.e@chula .ac.th; Chuchaat.t@chu.ac.th

Abstract: This work, characterizations of single human hairs by the Ge μIRE was introduced. The dome shape Ge μIRE is an accessory for ATR FT-IR spectral acquisition using an infrared microscope. Since the contact area of the Ge μIRE is small (100x100 μm), a small sample can be analysed. The chemical information and surface information of single human hairs were achieved. The observed spectra show the different spectral features between untreated hairs and chemical-treated hairs and cosmetic on hairs. The spectra acquired by the Ge μIRE were similar to those acquired by the conventional ATR technique. The spectrum intensity of spectra acquired by the Ge μIRE is 10 times better than those obtained by the conventional ATR due to the better contact. The spectra acquired by the Ge μIRE can be applied to forensic analysis.

C4_C0164 Synthesis and Charecterization of tetra(2-thienyl)porphyrin-metal(II)

Kanokrat Singoui[1*], Phimphaka Harding[2],Sorasak Danworaphong[1], and David Harding [2]

[1] Experimental Physics Research Unit, School of Science, Walailak University, 222 Thaiburi, Thasala District Nakhonsithammarat, Thailand. 80160
E-mail: s_kanokrat@hotmail.com Tel. (075) 673295

[2] Department of Chemistry, School of Science, Walailak University, 222 Thaiburi, Thasala District Nakhonsithammarat, Thailand. 80160

Abstract: The synthesis of 5, 10, 15, 20-tetra(2'-thienyl)porphyrin, T(2'-thio)P has been achieved by modification of the procedure for the synthesis of T(3'-thio)P. Yields are typically greater than 30%. The reaction of the porphyrin and appropriate divalent metal precursors yield the metalloporphyrin complexes, [MT(2'-thio)P] (M = Ni (**1**), Co (**2**), Mn (**3**), Zn (**4**), Cu (**5**)). The IR spectra show a new band at 945-990 cm^{-1}, typical of metal-nitrogen stretch. UV-Vis spectroscopic data reveal a red shift of 5 nm compared with the free porphyrin. Electrochemical studies confirm one-electron oxidations and reductions.

C4_C0166 INTERACTION OF H_2 MOLECULE WITH AROMATIC DICARBOXYLATE IN METAL ORGANIC FRAME WORK

Chutiparn Lesvachilapaiboon[1], Amonrat Sansureerangsikul[1], Chinapong Kritayakornupong[1], Supot Hannongbua[2]

[1] Department of Chemistry, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok, Thailand. E-mail: chinapong.kri@kmutt.ac.th Fax: (662)470-8843

[2] Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, Thailand.

Abstract: Interaction between H_2 molecule and aromatic dicarboxylates of metal organic framework (MOF) has been determined by employing the HF, B3LYP methods and using 6-31g(d) basis set. The individual linkers considered are1,4-benzenedicarboxylate (BDC), 1,3,5-tris(4-carboxyphenyl)benzene (BTB), and trigonal benzene-1,3,5-tricarboxylate (BTC). Various adsorption positions are evaluated for BDC, BTB, and BTC linkers. The most stable configuration of H_2 on BDC linker places the H_2 molecule above the aromatic plane with the axis pointing toward the middle of the ring. Among the considered dicarboxylate linkers, the largest interaction energy is found for BTB linker.

C4_C0168 Synthesis and Photophysical/Photochemical Characterization of Cinnamates

Thitinun Monhaphol[1], Bo Albinsson[2] and Supason Pattanaargson[1]

[1] Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330 Thailand.

[2] Department of Chemical and Biological Engineering/Physical Chemistry, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden.

Abstract: Five different substituted positions of 2-ethylhexyl-methoxycinnamates were synthesized and photophysical behavior of these cinnamates both trans- and cis-configuration were studied. The absorption spectrum of *para*-methoxycinnamate displays a single band which is similar to 2,4,6-trimethoxy substitution of cinnamate. However, as a consequence of spitting of excited singlet electronic configuration, the meta and ortho isomers display two less intense bands which is similar to 2,4,5-trimethoxy substituted one. In addition, ortho, meta and 2,4,5-substituted cinnamate are fluorescence but para and 2,4,6-substituented one show very weak fluorescence, therefore they can be deactivated through non-radiative pathway. The meta substituted one has longer singlet lifetime whereas the para and the 2,4,6-substituted cinnamate have very short lifetime (<10 ps). The torsion barrier for singlet state torsion of the meta and 2,4,5-substituted cinnamate are higher than ortho, para and 2,4,6 substituted one. This the large barriers for singlet state torsion in meta and 2,4,5 substituted cinnamate resulting from greater stabilization of singlet excited state ($^1S^*$). For the ortho, para and 2,4,6 substitued one, resonance stabilization of perpendicular excited singlet state ($^1P^*$) is expected.

C4_C0170 Design and Fabrication of a Mirror – Free Single Reflection ATR Accessory

Prompong Pienpinijtham, Taweesak Janduang, and Sanong Ekgasit
Sensor Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
E-mail: prom_gong@hotmail.com

Abstract: Attenuated Total Reflection (ATR) is an infrared spectroscopic technique based on sample absorption - occurs when infrared ray totally reflects at the surface of the internal reflection element (IRE) and sample. Commercial ATR accessory normally have plain or curve mirrors for coupling light into sample and collecting light to detector. These mirrors make accessory big and expensive. In single refection system, IRE must be hemispherical or triangular which is difficult to produce and expensive. Then design and fabrication of a mirror - free single reflection ATR accessory changes IRE shape to be parallelogram that allows incident beam and reflection beam to be in parallel. From the theoretical calculation, the most efficient parallelogram angle (θ) is 45°. Standard compound spectra collected by the novel accessory have the same quality as those from the commercial accessory. The novel accessory is reduced in size and prize because it dose not employ mirrors and hemisphere prism.

C4_C0187 DEALUMINATION STUDY OF ZEOLITE Y BY HCl METHOD

Chutima Thongkasam[1], and Kunwadee Rangsriwatananon

[1] School of Chemistry, Institute of Science, Suranaree University of Technology, 111 University Avenue, Sureenaree, Muang, Nakhon Ratchasima 30000 Thailand

E-mail:tchutima@hotmail.com, thongkasam@yahoo.com Phone:66(44)224-639, 66(1)063-2909 Fax:66(44)224-185

Abstract: The aim of this work is to study the dealumination method of zeolite Y by HCl method. Synthesis of zeoliteY was hydrothermally reacted with molar ratio of $4.62Na_2O : Al_2O_3 : 10SiO_2 : 180\ H_2O$ at 100°C. The obtained zeoliteY with Si/Al ~ 7.4 was used as the parent zeoliteY. The physicochemical properties of the zeolite Y samples before and after dealumination were characterized by X-ray Powder Diffraction Spectroscopy, X-ray Fluorescence Spectroscopy, Fourier Transform Infrared Spectroscopy, Differential Thermal Analysis and Scanning Electron Microscope measurements. The HCl dealumination method was performed by ion exchange of NaY into NH_4Y with NH_4NO_3 or NH_4Cl. Then NH_4Y was changed into HY form by calcinations at 500°C. It was found that NH_4NO_3 can promote to form HY better than NH_4Cl. These may be resulted from Cl^- that can damage the zeoliteY framework. In the dealumination process, HY form was dealuminated by HCl with concentration range of 0.01-0.3M. It was found that at 0.3M HCl concentration zeolite Y became amorphous phase. The highest Si/Al ratio with this method was about 8.9 and a percentage of crystallinity about 15% compared to parent zeoliteY. Therefore, the use of HCl method to dealuminate zeolite Y provided only low silica zeolite.

C4_C0188 THE RELATIONSHIP BETWEEN BINDING ENERGIES OF HIV-1 RT AND NNRTIs AND BIOACTIVITIES IN AIDS PATIENTS BY USING MOLECULAR DYNAMICS SIMULATION

Thanyarat_Udommaneethanakit[1], Panita Decha[1], Pathumwadee Intharathep[1],
Pornthep Sompornpisut[1] and Vudhichai Parasuk[1]

[1] Department of Chemistry, Faculty of Science, Chulalongkorn University, Phyathai Road, Bangkok 10330, Thailand. E-mail:Thanyarat22@yahoo.com, Fax: (662)218-7603

Abstract: Reverse trascriptase (RT) is one of main targets for anti-AIDS drugs. There are two classes of anti-HIV-RT drugs. The first class is nucleoside reverse transcriptase inhibitors (NRTIs) such as (AZT), lamivudine (3TC), stavudine (d4T) and the second class is non-nucleoside reverse transcriptase inhibitors (NNRTIs) such as efavirenz (EFV) and nevirapine (NVP). In the study, we performed a series of molecular dynamics simulations (MD) of the wild-type and fifty mutants HIV-1 RT complexed with efavirenz and nevirapine. All 50 mutant structures were constructed using amino acid sequences from Stanford HIV Drug Resistant Database and homology modeling technique. The binding energy of HIV-1 RT complex with inhibitors was calculated using Molecular Mechanic and Poisson-Boltzmann Solvent Accessible Surface Area (MM-PBSA) approach in order to compare with the biological activities. Binding energy differences between the mutant and the wild-type complexes show a poor correlation with the experimental data. However, the drug resistant predictions are in good agreement with the experiment. The discrepancy probably comes from the fact that the entropy and solvent effect have not yet been evaluated. In our further investigations, these values will be included and we are confident that the predicted binding energies will be greatly improved.

C4_C0201 The Alterations of the Adenine-Thymine Base Pairs on Interactions with Neutral and Charged Gold Atoms

Pipat Khongpracha[1,2], Panvika Pannopard, Kornvika Tangpong, Jumras Limtrakul[1,2*]

[1] Laboratory for Computational & Applied Chemistry, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

[2] Center of Nanotechnology, Kasetsart University Research and Development Institute, Kasetsart University, Bangkok 10900, Thailand

[*] Corresponding author: Tel. 662-5705047, Fax 662-942-8900 ext 324, E-mail: jumras.l@ku.ac.th

Abstract: The interactions of a Watson-Crick (WC) adenine-thymine (A-T) base pairs with an Au atom, Au^+ cation and Au^- anion are investigated by means of density functional theory method (B3LYP/6-31G(d,p)). Au^+ weakens the strength of N1-N3 hydrogen bonding but strengthens the O4-N6 hydrogen bonding in the T-A base pairing. The interaction performs in a similar manner with Au^0 but conversely with Au^-. The interaction energies of the thymine base with the adenine base bound with Au^0, Au^+ and Au^- are -13.305, -18.216 and -9.666 kcal/mol, respectively.

C4_C0215 THE HYDRATION REACTION OF CYCLOHEXENE OVER H-ZSM-5 ZEOLITE: A QM/MM STUDY

Karan Bobuatong[1,2], Jumras Limtrakul[1,2*]

[1] Laboratory for Computational & Applied Chemistry, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

[2] Center of Nanotechnology, Kasetsart University Research and Development Institute, Kasetsart University, Bangkok 10900, Thailand

[*] Corresponding author: Tel. 662-5705047, Fax 662-942-8900 ext 324, E-mail: jumras.l@ku.ac.th

Abstract: H-ZSM-5 zeolite was investigated theoretically by means of ONIOM2 (B3LYP/6-311G(d,p):UFF). The zeolite nanostructured pores included by the ONIOM method play an important role in regulating the orientation of the adsorbing molecule around the active site and significantly affect the energetic of the complexes. The hydration of cyclohexene catalyzed by H-ZSM-5 zeolites gives two different reaction mechanisms; both stepwise and concerted reaction mechanisms of the hydration reaction are considered. For the stepwise reaction mechanism, the hydration starts with the protonation of the adsorbed cyclohexene by the H-ZSM-5 zeolite leading to the formation of the alkoxide intermediate and, subsequently, the cyclohexanol can be generated by interaction with a water molecule. In the concerted reaction mechanism which is considered to be the reaction rate-determining step, the hydration of cyclohexene takes place in a single reaction step

without prior alkoxide oxide formation. The estimated activation barrier of rate-determining step and the reaction energiy are 16.26 kcal/mol and -7.4 kcal/mol comparable with experimental results of 16.85 kcal/mol and -8.9 kcal/mol, respectively. The results of this study is to provide data that will assist in understanding how the hydration of cyclohexene over H-ZSM-5 zeolite works.

C4_C0216 THE EFFECT OF THE FINITE LENGTH AND TYPE OF SINGLE-WALLED CARBON NANOTUBES CAPPED WITH FULLERENE HEMISPHERES ON THEIR ELECTRONIC PROPERTIES AND CHEMICAL REACTIVITY VIA 1,3-DIPOLAR CYCLOADDITION OF OZONE

Montree Sawangphruk[1,2], Tanin Nanok[1,2], Supawadee Namuangrak[1,2], Piboon Pantu[1,2], Jumras Limtrakul[1,2*]

[1] Laboratory for Computational & Applied Chemistry, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

[2] Center of Nanotechnology, Kasetsart University Research and Development Institute, Kasetsart University, Bangkok 10900, Thailand

[*] Corresponding author: Tel. 662-5705047, Fax 662-942-8900 ext 324, E-mail: jumras.l@ku.ac.th

Abstract: The 1,3-dipolar cycloaddition (1,3-DC) of ozone on the cap of [5,5]-armchair single-walled carbon nanotubes ([5,5]-ASWNTs) and [9,0]-zigzag single-walled carbon nanotubes ([9,0]-ZSWNTs) has been carried out using a PBE/def-SV(P) method as compared with an ONIOM(B3LYP/6-31G(d):AM1) approach. Increasing of the length of SWNTs leads to the change of electronic properties. The absolute chemical hardness of [5,5]-ASWNTs, calculated using the appropriate PBE approach, fluctuates and decreases from 0.83 eV to 0.15 eV for C_{60} to C_{200}. These of [9,0]-ZSWNTs decreases without fluctuation from 0.72 eV to 0.28 eV for C_{78} to C_{204}. Also, the FMO Interaction energy of [5,5]-ASWNTs decreases with the fluctuation behavior from 0.05 eV to -1.05 eV. For [9,0]-ZSWNTs, it decreases from -0.02 to -0.94 eV. On the contrary, their activation and reaction energies are insensitive to the length and type of nanotubes. The basis set super position error (BSSE) corrected activation energies are 2.29, 2.16-2.26, and 2.15-2.18 kcal/mol and the chemisorption energies are exothermic by 44.56, 45.02-46.86, and 48.21-48.53 kcal/mol for C_{60}, [5,5]-ASWNTs, and [9,0]-ZSWNTs, respectively.

C4_C0219 The Adsorption and Diffusion of 1-Butene and cis-2-Butene on H-FER: Combined Quantum Mechanics/ Molecular Mechanics and Molecular Dynamics Simulation

Bundet Boekfa[1,2], Jumras Limtrakul[1,2*]

[1] Laboratory for Computational & Applied Chemistry, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

[2] Center of Nanotechnology, Kasetsart University Research and Development Institute, Kasetsart University, Bangkok 10900, Thailand

[*] Corresponding author: Tel. 662-5705047, Fax 662-942-8900 ext 324, E-mail: jumras.l@ku.ac.th

Abstract: The adsorption and diffusion of 1-butene and cis-2-butene have been studied by means of combined Quantum Mechanics/Molecular Mechanics and Molecular Dynamics Simulation. The interaction energies are calculated to be -16.55 and -14.13 kcal/mol for 1-butene and cis-2-butene, respectively with combined Quantum Mechanics/Molecular Mechanics. This trend agrees with the interaction energies from MD simulation in the order 1-butene more than cis-2-butene. The diffusion activation energies from the MD simulation are 5.11 and 5.06 kcal/mol for 1-butene and cis-2-butene, respectively. The results correlate well to the experimental observation.

C4_C0228 Confinement Effects on Adsorption and Diffusion of Hexane in Nanoporous MCM-41 with Different Pore Sizes: a Molecular Dynamics Study

Winyoo Sangthong[1,2], Jumras Limtrakul[1,2*]

[1] Laboratory for Computational & Applied Chemistry, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand

[2] Center of Nanotechnology, Kasetsart University Research and Development Institute, Kasetsart University, Bangkok 10900, Thailand

[*] Corresponding author: Tel. 662-5705047, Fax 662-942-8900 ext 324, E-mail: jumras.l@ku.ac.th

Abstract: Molecular Dynamics (MD) simulations were utilized to study the adsorption and diffusion of hexane in four different pore sizes siliceous MCM-41 at 300K. The calculated adsorption energies obtained found to be in good agreement with experimental ones for the same pore sizes. As a result of confinement in MCM-41, the free energies adsorption of hexane increase when the pore sizes decrease and increase also with the loadings. The calculated self-diffusion coefficients of hexane decrease with increasing loadings and they decrease if the pore sizes decrease, which, again, are reasonably close to the available experimental data. The average distances between the centers of the mass of hexane molecules in the smallest pores are only marginally less than in the larger pores and of those in the liquid phase. It was further found that for low loadings the hexane molecules lie parallel to the pore channel for every pore sizes. When the loadings are increased, they build up concentric rings with sizes depending on the pore channel diameters. Hexane molecules in the larger models behave in a similar manner to those in the liquid phase.

C4_C0229 EFFECTS OF MUTATIONS ON THE SUSCEPTIBILITY OF OSELTAMIVIR TO INFLUENZA A VIRUS N1 NEURAMINIDASE AS STUDIED BY MOLECULAR DYNAMICS SIMULATIONS

Panita Decha[1], Maturos Malaisree[1], Onjira Aruksakunwong[1], Supot Hannongbua[1]
[1] Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.
E-mail:panita487@hotmail.com, Tel: (662)218-7602-4, Fax: (662)218-7603

Abstract: Oseltamivir (OTV) is a potent and specific inhibitor of influenza neuraminidase (NA). However, an influenza A virus subtype H5N1was found to reduce susceptibility to oseltamivir via I222T, H274Y and double I222T/H274Y mutations by a factor of 2, 10 and 1000, respectively. To understand the source of drug resistance due to these mutations in molecular level, molecular dynamics simulations (MD) were carried out for the three complexes, OTV-I222T, OTV-H274Y and OTV-I222T/H274Y. In our previous work, two of bulky side chains of OTV-wild type complex, N-acethyl (–NHAc) and 1-ethylproxy group (–OCHEt2), were observed to rotate in order to adjust its size to fit into the N1 catalytic site in comparison to that in the OTV-N2 and OTV-N9 complexes. The MD results for the OTV-mutations complexes show that both side chains were turned back to their original position. Interestingly, OTV-enzyme interactions in the OTV-mutations are weaker than that of the OTV-wild type. Furthermore, the calculated ligand/enzyme binding free energies of -8.56, -5.52 and -2.02 kcal/mol agree totally with the experimental inhibitory activities of 2, 10 and 1000 resistant folds for the OTV-I222T, OTV-H274Y and OTV-I222T/H274Y complexes, respectively.

C4_C0239 EFFECT OF AMINE SUBSTITUTED ITQ-24 ZEOLITE ON THE PROTONATION OF ALKENE: A QM/MM STUDY

Bavornpon Jansang[1,2] Pipat Khongpracha[1,2] and Jumras Limtrakul[1,2*]
[1] Laboratory for Computational & Applied Chemistry, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand
[2] Center of Nanotechnology, Kasetsart University, Bangkok 10900, Thailand
E-mail address: bavornpon@yahoo.com (B. Jansang), pipat_k@msn.com (P Khongpracha) and fscijrl@ku.ac.th (J. Limtrakul).

Abstract: The alkoxide formation of ethylene over amine-substituted and non-substituted in the ITQ-24 zeolite framework have been computed within the framework of the ONIOM approach utilizing the two-layer ONIOM scheme (B3LYP/6-31G(d,p): UFF). Amine substitution reduces the apparent activation energy of the reaction form 17.34 to 12.40 kcal/mol. The results imply that amine substitution in zeolite framework enhances the basicity of the system.

C4_C0240 MOLECULAR DYNAMICS SIMULATION OF SOLUTION OF SODIUM IONS IN LIQUID AMMONIA

Teeranan Nongnual[1], Tawun Remsungnen[2]
[1] Department of Chemistry, Faculty of Science, Prince of Songkla University, Hatyai, Songkhla 90112, Thailand.
E-mail: gangurru@gmail.com
[2] Department of Mathematics, Faculty of Science, Khonkaen University, Khonkaen 40002, Thailand.

Abstract: The results of molecular dynamics simulation of sodium-ammonia solution using three-body potential functions for high concentration, 19.6 MPM at 264.18 K, are reported. The system consisted of 50 sodium ions, 50 free electrons and 205 ammonia molecules. The results show the random position of the input in a periodic box would be clusters of sodium ions in the solution after the dynamics simulation; 10 ps after equilibrium. The position and solvation of sodium in solution are described by radial distribution functions (RDFs).

C4_C0257 THE 3D SOLUTION STRUCTURE AND STEREOCHEMISTRY DETERMINATION OF SMALL FLEXIBLE ORGANIC MOLECULES BY CONFORMER POPULATION ANALYSIS

Panichakorn Jaiyong[1], Ekasith Somsook[2], Shuleewan Rajviroongit[2]
[1] Department of Chemistry, Faculty of Science and Technology, Thammasat University, Pathum Thani, Thailand.
E-mail:scpj@tu.ac.th, Fax: (662)564-4483
[2] Department of Chemistry, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok, Thailand.

Abstract: The three-dimensional solution structure and the stereochemistry of flexible diastereomers, so-called *Methyl11- [2- ([1- (methoxycarbonyl)-2-1[1- (methoxycarbonyl)vinyl]cyclopropyl}carbonyl)cyclopropyl] -9, 10- dihydro -9, 10 ethanoanthracene-11-carboxylates*, were determined via a comparison between the quantified nuclear relaxations from 2D-^{1}H NMR spectroscopy (NOESY) and the simulated values from the full relaxation matrix approach by using a multiconformational algorithm, Conformer Population Analysis. The computational results showed that the best preferred structure of a major isomer adopted in solution as a single conformation with the chirality SRRRR and the R-factor of 0.612. Only one of its chiral carbons was probably changed during a thermal reaction to form a weak interaction for the increased stability. The other major isomer was proposed to posses the R chirality for all asymmetrical carbons with the R-factor of 0.613 as a single conformation. It was possible to adopt the mixture of two or three conformations with the percentage ratio 66:34 (R-factor = 0.594) and 38:38:24 (R-factor = 0.583), respectively.

C4_C0258 Vibrational spectroscopic study of $AlPO_4 \cdot H_2O$ by deuterium isotopic dilution technique

Banjong Boonchom[1], Sujittra Youngme[2] and Chanaiporn Danvirutai*
[1,2,*] Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.

Abstract: Al(III)PO_4•H_2O and its deutearated analogues have been synthesized and investigated by FT-IR and FT-Raman spectroscopy. Vibrational bands are identified in relation to the crystal structure in terms of the fundamental vibrating units namely PO_4^{3-}, H_2O, AlO_4 and AlO_6. The vibrational modes of PO_4^{3-} ion and H_2O molecules are analyzed based on the correlation field splitting. Three FTIR bands of OH stretching of HOH are observed at 3447, 3369, and 3121 cm^{-1}. The band at 3369 cm^{-1} is assigned to weakly hydrogen bonded water and the band at 3121 cm^{-1} to strong hydrogen bonded water. The OD stretching bands of deuterated analogues are observed at 2551, 2499 and 2376 cm^{-1} which resemble the spectral profile of OH stretching of HOH region. Two HOH bending are observed at 1662, 1639 cm^{-1} and HOD bending at 1491, 1455 cm^{-1}. These doublet bands indicate two types of water molecules with different hydrogen bonding strengths. The bands at 3369 and 3121 cm^{-1} lead to the estimation of $R_{O_w\ O}$ by using a Libowitzky type function that found to be 2.778 and 2.680 Å. The correlation function for the estimation is in the form $\nu_1 = 3592 - 304 \times 10^9 \exp(R_{O_w\ O}/0.1321)$, $R^2 = 0.96$ [Libowitzky, 1999].

C4_C0259 CONFORMATIONAL ANALYSIS OF HIV-1 REVERSE TRANSCRIPTASE INHIBITOR(S)-6-CHLORO–4-(CYCLOPROPYLETHYNYL)-1,4–DIHYDRO-4-(TRIFLUOROMETHYL)-2H-3,1-BENZOXAZIN-2-ONE (EFAVIRENZ) AND ITS DERIVATIVES, BY USING QUANTUM CHEMICAL CALCULATIONS

Auradee Punkvang[1*], Patchareenart Saparpakorn[2], Supa Hannongbua[2] and Pornpan Pungpo[1]
[1] Department of Chemistry, Faculty of Science, Ubonratchathani University, Ubonratchathani, 34190
[2] Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, 10900
E-mail address: Punkvang@yahoo.com

C4

Abstract: Conformational analysis of HIV-1 reverse transcriptase inhibitor (s)–6-chloro–4-(cyclopropylethynyl)-1,4–dihydro-4-(trifluoromethyl)-2H-3, 1-benzoxazin-2-one (efavirenz) and its derivatives (the best compounds active against WT and K103N HIV-1 RT) were investigated based on various methods of quantum chemical calculations, AM1, PM3, HF/3-21G, HF/6-31G* and B3LYP/6-31G*. The starting geometry of efavirenz was taken from X-ray crystallographic data. The rotational potentials along the single bond between the cyclopropylethynyl group and atoms in the heterocyclic ring (alpha dihedral angle) for all derivatives were examined. Moreover, the rotational potentials of the methoxy side chain to the heterocyclic ring system (beta dihedral angle) were also considered. The comparison of the calculated energy minimum conformations with the X-ray HIV-1 RT/efavirenz complexed structure and the docked conformations derived by docking calculations. The results show that based on HF and B3LYP calculations, the energetical favorable conformers were found at the similar regions, whereas AM1 and PM3 calculations seem to be not accurate enough to obtain helpful information of conformational analysis of this molecules. For the alpha dihedral angles of efavirenz derivatives, the energetical favorable conformation obtained from B3LYP/6-31G* show high correspondence to the conformation in the X-ray crystallographic structure, whereas the energy minimum conformer obtained from HF/3-21G is good agreement with the docking conformer. Whereas, for the beta dihedral angle, it is interesting to note that an energy minimum conformation obtained from B3LYP/6-31G* calculation is the most similar to the docking conformer. Consequently, the comparative conformational analysis provide beneficial information concerning the conformational possibilities and the range of flexibility which is related to the biological behaviors of efavirenz derivatives to inhibit WT and K103N HIV-1 RT.

C4_C0265 Theoretical study of structure and energetic of a novel pyrrolidinyl PNA binding to DNA

Khatcharin Siriwong,[a*] Parawan Chuichay,[b] Suwipa Saen-oon,[c] Tirayut Vilaivan[c] and Supot Hannongbua[c]
[a] Department of Chemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand
[b] Department of Physics, Faculty of Science, Kasetsart University, 50 Phahon Yothin Road, Cha-tuchak, Bangkok 10900, Thailand
[c] Department of Chemistry, Faculty of Science, Chulalongkorn University, Phayathai Road, Patumwan, Bangkok 10330, Thailand

Abstract: -Molecular dynamics (MD) simulations have been used to study the structure of a novel pyrrolidinyl PNA binding to DNA (PNA×DNA) for both parallel and antiparallel configurations in aqueous solution. A DNA duplex (DNA×DNA) was also carried out for comparison. B-like form was used as a model for all starting structures. MD trajectories were generated for 2 ns using AMBER 8 package. Furthermore, Molecular Mechanics-Generalized Born/surface area (MM-GBSA) approach and normal-mode analysis have been used as the postprocess to evaluate the binding free energy of the double strand. As a result, the trajectories show a stability of duplexes during the simulation time period. Both DNA×DNA and PNA×DNA(antiparallel) duplexes remain in canonical B as their starting structures, whereas a distortion from B-like is observed in PNA×DNA(parallel) duplex. As shown by the radial distribution function, the distance of the first solvation shell of PNA strand is larger than that of DNA strand because of a hydrophobic property of PNA. MM-GBSA result shows that PNA×DNA(antiparallel) is the most stability and parallel fashion is more stable than DNA duplex, which are in agreement with the experimental data.

C4_C0266 THEORETICAL INVESTIGATIONS ON STRUCTURAL ELECTRONIC AND OPTICAL PROPERTIES OF CARBAZOLE-CAPPED MOLECULES AS NOVEL BLUE LIGHT-EMITTING HOLE-TRANSMITTING MATERIALS, BASED ON QUANTUM CHEMICAL CALCULTIONS

Pornpan Pungpo[1*], Songwut Suramitr[2] and Siriporn Jungsuttiwong[1]
[1]Department of Chemistry, Faculty of Science, Ubonratchathani University, Ubonratchathani, 34190
[2]Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, 10900
E-mail address: pornpan_ubu@yahoo.com

Abstract: The conformational analysis and electronic properties for carbazole–capped molecules as novel blue light-emitting

hole-transporting materials shown as models A and B (Figure 1) were investigated by using various quantum chemical calculations. The conformational analysis were carried out based on AM1, PM3, HF/3-21G* and B3LYP/6-31G* calculations. The torsional energy potential along C4-N21-C22-C23 dihedral angle (alpha angle) and C38-C40-N63-C44 dihedral angle (beta angle) were examined. The results show that AM1 and PM3 results are not accurate enough to obtain helpful information for the conformational analysis of these models. Based on HF/3-21G* and B3LYP/6-31G* results, the preferable energetic conformers for both models with alpha angle at 90 degree and beta angle at 90 degree were found for model A. The alpha and beta angles of the lowest energy conformers of model B are 60 degree and 300 degree, respectively. The results reveal that the perpendicular form is preferred for both models A and B due to strong steric interaction between two units, as shown. To determine the electronic properties of models A and B, the B3LYP/6-31G* conformers obtained from conformational analysis were used to compute the energies of highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO) at B3LYP/6-31G* level of the calculations. The calculated energy band gaps of models A and B are 3.77 eV and 3.31 eV, respectively. The obtained results are in good accordance with the energy band gap derived from the experimental data (3.50 eV and 3.35 eV for models A and B, respectively). In summary, the calculated structural and electronic properties can be applied as fundamental guideline in designing novel conducting polymer materials.

C4_C0267 THE DFT STUDY OF INTERACTION OF Au CLUSTERS AND RUTILE (110) SURFACES

Piti Treesukol[1], Jumras Limtrakul[2] and Thanh N. Truong[3]
[1] Faculty of Liberal Arts and Science, Kasetsart University, Kampaeng Saen, Nakorn Pathom, 73140, Thailand
[2] Faculty of Science, Kasetsart University, Bangkok, 10900, Thailand
[3] Henry Eyring Center for Theoretical Chemistry, Chemistry Department, University of Utah, Salt Lake City, UT 84112

Abstract: Highly dispersed gold particles on reducible TiO_2 can exhibit surprisingly high catalytic reactivity for CO oxidation reaction. The interaction of Au clusters with TiO_2 rutile (110) surface has been studied by an embedded cluster model at DFT/B3LYP level of calculation. Small Au clusters, which have been proposed to function as an active center for CO oxidation, can be stabilized on the TiO_2 surface by O-vacancy. The binding energy of an Au atom to the defective surface is 50 kcal/mol while that to the perfect surface is about 18 kcal/mol less. The electron density of the Au atom increases significantly due to the electron-transfer from the vacancy site. The electronic properties of the TiO_2 surface is found to be perturbed by the Au cluster as well. The electron density of the surface 5-fold Ti atoms next to the vacancy site increases significantly due to the adsorption of Au, which can enhance the ability in activating adsorbates such as O_2 which is the reason why Au/TiO_2 interface has an important role in the oxidation of CO.

C4_C0279 RAMAN AND INFRARED SPECTROSCOPIC STUDIES OF DIVALENT CATION PHOSPHATE HYDRATES RELATED TO SALINE SOIL

Chanaiporn Danvirutai[1*], Chanugorn Tabtimsai[1], and Tipaporn Srithanratana[1]
[1*, 2, 3] Department of Chemistry, Faculy of Science, Khon Kaen University, Khon Kaen 40002 , Thailand.
E-mail address: chanai@kku.ac.th, chanugorn_tabtim@hotmail.com

Abstract: The intermolecular interaction in divalent cation phosphate hydrates related to saline soil were studied for $Mg_3(PO_4)_2 \cdot 8H_2O$ (bobierrite) and $MgHPO_4 \cdot 3H_2O$ (newberyite) that isostructure with $Fe_3(PO_4)_2 \cdot 8H_2O$ (vivianite) and $MnHPO_4 \cdot 3H_2O$, by Raman and Infrared Spectroscopy and isotopic dilution technique. The observed OH stretching of water in phosphate hydrates and uncoupled ν_{OH} (HOD) vibration in D_2O condition lead to the estimation of the intermolecular distance between oxygen water and anion oxygen ($R_{O...O}$) and enthalpy of hydrogen bonding ($-\Delta H_H$) by using equation $R_{O...O} = 3.764 - 0.169\ln(\Delta\nu_{OH}\ /cm^{-1})$ Å and $-\Delta H_H = 1.286 - 0.0418(\Delta\nu_{OH}$ HOD/ $cm^{-1})$ kJ/mol, respectively. The $R_{O...O}$ and $-\Delta H_H$ for $Mg_3(PO_4)_2 \cdot 8H_2O$, $MgHPO_4 \cdot 3H_2O$, $Fe_3(PO_4)_2 \cdot 8H_2O$ and $MnHPO_4 \cdot 3H_2O$ were found to be 2.733, 2.790, 2.707, and 2.751 Å and -17.375, -20.510, -12.011, and -15.410 kJ/mol OH, respectively. The mole number of water of crystallization of octahydrate and trihydrate were studied by thermochemical and Karl-Fischer methods, and found to be 8 and 3 moles, respectively. The phosphate hydrates prepared from the variation of cation mole ratios; Fe(II)/Mg(II) and Mn(II)/Mg(II) in 5 categories, 1:1, 1:2, 1:3, 2:1 and 3:1 were studied. The data from FT-IR showed the spectrum characterized for $Fe_3(PO_4)_2 \cdot 8H_2O$, $MnHPO_4 \cdot 3H_2O$, (Mg, Fe)$_3(PO_4)_2 \cdot 8H_2O$, (Mg, Mn)$HPO_4 \cdot 3H_2O$. Moreover, the effects of ionic strength approximating salinity levels on the precipitation of compounds were investigated. Initial pH of the phosphate hydrates preparations were followed up for four salinity levels. It was found that the initial pH for those 4 phosphate hydrates is as follow: $S_{ns} < S_{gs} \approx S_{ms} \approx S_{vs}$.

C5_C0005 Rotenoids from Leaves of *Millettia brandisiana*.

Chiangmai, 50200, Thailand.
Anan Athipornchai[1], Orasa Pancharoen[1], Channarong Choowong[1], Lampa Yossombat[1], Ampai Panthong[2]
[1] Department of Chemistry, Faculty of Science, Silpakorn University, Nakorn Pathom, 73000, Thailand.
[2] Department of Pharmacology, Faculty of Medicine, Chiangmai University,

Abstract: Chromatographic separation of the ethyl acetate extract from leaves of *Millettia brandisiana* led to the isolation of three isoflavones : toxicarol isoflavone (1), robustigenin (2) and 5,7,2′,5′-tetramethoxy-4′-γ,γ-dimethylallyloxyisoflavone (11); four rotenoids : α-toxicarol (3), semundone (4), 12a-hydroxy-α-toxicarol (5) and 6-deoxyclitoriacetal (6); four dehydrorotenoids : 6a,12a-dehydro-α-toxicarol (7), 6a,12a-dehydrosermundone (8), 6-hydroxy-6a,12a-dehydro-α-toxicarol (9) and stemonal (10) together with 3-*O*-[β-D-glucopyranosyl]-sitosterol (12). The structures of isolated compounds were identified by spectroscopic methods. In addition, compound 5 showed higher anti-inflammatory activity than that of phenylbutazone.

C5_C0012 Effect of Extracts from Some Local Plants on Spodoptera litura F.

Vanida Chairgulprasert Pintip Jantharatep and Kittipong Longsa

[1] Department of Science, Faculty of Science and Technology, Prince of Songkla University, Pattani Campus, 94000

[2] Department of Technology and Industry, Faculty of Science and Technology, Prince of Songkla University, Pattani Campus, 94000

Abstract: Various crude extracts including hexane, dichloromethane and methanol extracts from leaves of *Melaleuca cajuputi, Litsea patiolata, Sterculia foetida, Curcuma aeruginosa* and rhizomes of *Curcuma aeruginosa* were studied for the mortality activity on *Spodoptera litura*. In preliminary test, three hexane crude extracts including leaves of *M. cajuputi, L. patiolata* and rhizomes of *C. aeruginosa* at the concentration of 50% (w/v) showed high potential to kill the 2nd stage larvae of *S. litura*. Further investigation on the efficacy of hexane crude extracts at various concentrations for 72 hrs, rhizomes of *C. aeruginosa* exhibited the highest insecticide activity for both feeding and topical tests with LC_{50}11% and 13%, followed by leaves of *M. cajuputi* with LC_{50} 28% and 27%. All three hexane crude extracts could inhibit oviposition of adult of *S .litura* on Chinese kale. Additionally, the hexane crude extract from rhizomes of *C. aeruginosa* performed the best activity to reduce the population of larvae of *S .litura*.

C5_C0045 High Performance Liquid Chromatographic (HPLC) Method for the Determination of Cephalexin, Cefazolin and Cefoxitin

Chalermporn Thongpoon[1], Boonsom Liawruangrath[2], Saisunee Liawruangrath[3], Theeraphan Machan[2] and Wisanu Thongchai[2]

[1] Program of Chemistry, Faculty of Science and Technology, Pibulsongkram Rajabhat University, Phitsanulok, 65000, Thailand.

[2] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai, 50200, Thailand.

[3] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, 50200, Thailand.
E-mail address: g4370029@yahoo.com, boonsom@pharmacy.cmu.ac.th

Abstract: A fast and reliable HPLC method has been developed for the simultaneous determination of cephalexin, cefazolin and cefoxitin in pharmaceuticals. Separation was achieved on an ODS Hypersil column C_{18} (4.6 mm x 125 mm, 5 µm) with UV detection at 254 nm. The mobile phase system was a mixture consisting of acetonitrile-10 mM phosphate buffer (12:88 % v/v) containing tetraethyl ammonium bromide (10mM) adjusted to pH = 4.5 with triethylamine or phosphoric acid. The mobile phase was pumped through the chromatographic system at a flow rate of 1 mL min^{-1}. The calibration curves for cephalexin, cefazolin and cefoxitin were linear over the ranges 0.1-20, 0.1-20 and 0.1-30 µg mL^{-1} with $r^2 > 0.999$. The LODs for cephalexin, cefazolin and cefoxitin were 0.02, 0.02 and 0.04 µg mL^{-1}, respectively. The method was successfully applied to the simultaneous determination of the three cephalosporin antibiotics in pharmaceutical formulations.

C5_C0046 DETERMINATION OF CURCUMINOID CONTENTS BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

Wisanu Thongchai[1], Boonsom Liawruangrath[1], Saisunee Liawruangrath[2], Chalermporn Thongpoon[3], Suwanna Saysin[1], Theeraphan Machan[1] and Chonlayut Raweewan[1]

[1] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai, Thailand. E-mail: wisanuthongchai@hotmail.com, Fax: (053) 222741

[2] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, Thailand.

[3] Program of Chemistry, Faculty of Science and Technology, Pibulsongkram Rajabhat University, Phitsanulok, 65000, Thailand.

Abstract: Curcuminoids are orange-yellow color pigments of turmeric. They consist of a mixture of three different curcuminoids, namely, curcumin, demethoxycurcumin and bisdemethoxycurcumin. These were isolated by preparative TLC and the curcuminoids were analyzed by HPLC. HPLC separation was performed on an analytical C_{18} column using methanol : 2% AcOH : acetonitrile (23:36:41, v/v/v) as mobile phase at a flow rate of 1.0 ml min^{-1}, with detection at 425 nm. Linear calibration curves of curcumin, demethoxycurcumin and bisdemethoxycurcumin were obtained over the concentration ranges of 7.82-156.31, 1.88-37.65 and 0.30-6.04 µg ml^{-1}, respectively. The average percentage recoveries of the method were in the ranges of 98.66-101.78. The method was successfully applied to the determination of three different curcuminoids content in different varieties of turmeric in local market samples. Chiang Mai market (two samples) and Phitsanulok market (three samples) were analyzed to detect the percentage of these three curcuminoids content. The percentages of curcumin, demethoxycurcumin and bisdemethoxycurcumin as estimated using their calibration curves were found to be 0.299-4.305, 0.318-2.320 and 0.273-1.851, respectively, in the five different samples. The proposed HPLC method was rapid, simple, selective and it is suitable for routine analysis.

C5_C0048 FREE FATTY ACIDS AND ANTITUBERCULOSIS ACTIVITY FROM *HELIOTROPIUM INDICUM* LINN.

Theeraphan Machan[1], Boonsom Liawruangrath[1], John Korth[2], Saisunee Liawruangrath[3], Apiwat Baramee[3], Stephen G. Pyne[2] and Chalermporn Thongpoon[3]

[1] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai 50200, Thailand.

[2] Department of Chemistry, University of Wollongong, Wollongong, NSW 2522, Australia.

[3] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.

[4] Program of Chemistry, Faculty of Science and Technology, Pibulsongkram Rajabhat University, Phitsanulok 65000, Thailand. E-mail address: tmachan@yahoo.com, boonsom@pharmacy.cmu.ac.th

Abstract: Sixteen free fatty acids from the crude hexane extract of *Heliotropium indicum* Linn. have been identified after conversion to their methyl esters with boron trifluoride-methanol followed by quantification by GC-FID and identification by GC-MS analysis. They accounted for 95% of the chromatographable components, with 9,12-octadecadienoic acid, (39.7%), 9-octadecenoic acid (32.4%), hexadecanoic acid (14.2%) and octadecanoic acid (5.1%), as the major constituents. A small amount of 6,10,14-trimethyl-2-pentadecanone and 3,7,11,15-tetramethyl-2-hexadecen-1-ol as well as a homologous series of n-alkanes present at trace level and ranging from C_{25} to C_{31} was also found. The crude hexane extract showed moderest antituberculosis activity (MIC of 100 µg/mL) against *Mycobacterium tuberculosis* H37Ra.

C5_C0052 Comparative of Hesperidin Contents in Pummelo and Mandarin Peel

Santiya Kerdphocha and Suwimon Ruengsri
Chemistry Program, Faculty of Science and Technology, Nakhon Pathom Rajabhat University, Nakhon Pathom, Thailand
E-mail: Suvimoln@npru.ac.th

Abstract: The hesperidin contents from pummelo and mandarin peel were investigated. Methanol was used as solvent in the ratio of 1:10 (g/mL) sample to solvent. The extract was divided equally for qualitative and quantitative analysis. The antioxidative activity was first analysed qualitatively. The extracted powders from pummelo and mandarin peel showed similar protection factor, at 1.33 in lard and 1.13 in coconut oil. The protective factor of the standard reference (BHA) was found to be 1.44 and 1.25 in lard and coconut oil, respectively. UV-VIS Spectrophotometer was used to determine the quantity of hesperidin in the extracts. Hesperidin contents in pummelo and mandarin peel extract were 24.20 ± 0.02 mg/g and 37.88 ± 0.37 mg/g, respectively. The results from UV-VIS spectrophotometer are in accordance to the qualitative data, indicating that the extracts from pummelo peel had lower contents of hesperidin than the mandarin peel.

C5_C0080 Antifungal activities of turmeric crude extract on the fish pathogenic fungi in vitro

Pareeya Udomkusonsri[1], Nampong Kongkathip[2], Boonsong Kongkathip[2], Sumaree Boonma[3], Kamonlchai Trongvanlchnami[1], Santi Kaewmokul[4], Napasorn Kusucharit[1]
[1] Department of Pharmacology, Faculty of Veterinary Medicine, Kasetsart University
[2] Department of Chemistry, Faculty of Science, Kasetsart University
[3] Department of Microbiology and Immunology, Faculty of Veterinary Medicine, Kasetsart University
[4] Department of Physiology, Faculty of Veterinary Medicine, Kasetsart University

Abstract: Crude ethanol extracts of turmeric (Curcuma longa Linn.) were studied for fungistatic and fungicidal activities against four fish pathogenic fungal isolates; Saprolegnia diclina, Saprolegnia parasitica H2, Achyla channae and Aphanomyces piscicida on Glucose Yeast Extract (GY) agar. 1% DMSO was used as diluent for antifungal test. Minimal inhibitory concentration (MIC) of turmeric crude against S. diclina, S. parasitica H2, A. channae and A. piscicida were 2,500, 2,500, 1,250 and 62.5 µg/ml, respectively. The fungicidal concentrations against S. diclina, S. parasitica H2, A. channae and A. piscicida were 5,000, 5,000, 5,000 and 625 µg/ml, respectively. This study showed that turmeric crude extracts had antifungal activity against those 4 water mold isolates.

C5_C0110 QUERCETIN: CHARACTERIZATION AND DEVELOPMENT OF LIPOSOMAL ENCAPSULATION FOR DRUG DELIVERY SYSTEM

Saengrawee Sutthiparinyanont[1], Aroonsri Priprem[1], and Malyn Chulasiri[2]
[1] Faculty of Pharmaceutical Sciences, Khon Kaen University, Khon Kaen, Thailand
[2] Research and Development Laboratories, SJI, Bangkok, Thailand

Abstract: Physicochemical studied of quercetin, an effective antioxidant, were carried out including solubility, stability, and antioxidant activity. The antioxidant activity was determined using 2,2-diphenyl-picryl hydrazine (DPPH) method. Quercetin was encapsulated in liposomal particles by thin-film hydration with ultrasonication and extrusion techniques. Characterizations of quercetin-liposomal particles including shape, size, surface charge, lipid forming, and encapsulation efficiency were performed. The results showed that solubility (3.80 and 4.00 mg/mL at 25 and 37 °C, respectively) and stability of quercetin were highest in alcohol. The degradation rate of quercetin was reduced rapidly upon initiation and converged after 12 hr. DPPH determination showed EC_{50} of quercetin of 0.012 mg, comparable with vitamin C and E. The encapsulation product has spherical negative charge particle with size in the range of 40-500 nm. Percentage of lipid forming and encapsulation efficiency were about 80% and 66%, respectively. It is expected that the quercetin encapsulation could be applied for drug delivery system used to protect oxidative stress caused of many chronic diseases.

C5_C0129 CHEMICAL CONSTITUENTS AND ANTIOXIDANT ACTIVITY OF *KAEMPFERIA PARVIFLORA* WALL. EX BAK.

Kamolporn Panyakard*, Sunee Chansakaow[1], Chaiyavat Chaiyasut[1]
*,[1]Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiangmai University

Abstract: Krachai-dum (*Kaempferia parviflora* Wall. ex Bak.) is used in traditional medicine as health-promoting herbs. The present study investigate chemical constituents and antioxidant activity of *K. parviflora*. Dry powder of the rhizomes was

extracted exhaustively with *n*-hexane, ethyl acetate, methanol and water, respectively. Then, the extracts were examined and assessed for antioxidant activity. Flavonoid compounds were found in *n*-hexane and ethyl acetate extracts whereas anthocyanins, flavones and phenolic compounds were found in alcohol extract. The highest antioxidant activity was found in alcohol fraction followed by ethyl acetate, water and n-hexane, respectively. Comparisons of antioxidant activity (*ABTS*[0] and *FRAP Assay*) between crude extracts and isolated compounds, it was found that crude extracts gave the better activities than isolated pure compounds. The results showed that chemical constituents and antioxidant activity of crude extracts depended upon extracting solvents and different flavonoids in each extract.

C5_C0132 Chemical constituents and effect on central nervous system of essential oil from Thai Citrus plants

Wanwisa Srinuanchai[1], Wirat Niwatananun[1], Pimporn Leelapornpisid[1], Suwanna Vejabhikul[1], Sunee Chansakaow[1]
[1] Department of Pharmaceutical Science, Faculty of Pharmacy Chiang Mai University, Chiang Mai 50200, Thailand.

Abstract: The objectives of this research were to study the chemical constituents and to investigate the effect of citrus oils from Thai Citrus plants on central nervous system (CNS) in rats. Among this study, there were 8 cultivar of Citrus (som sai nam peung, som sweet mandarin, som ocean, som king, som jug, som o thong dee, som o kao nam peung and grapefruit). The essential oils of Citrus peel were obtained by direct steam distillation. The volatile components of the peel oils were quantitatively and qualitatively determined by GC and GC/MS. Limonene (86.41-96.72%) was the major compound followed by myrcene (1.51-1.79%), and α-pinene (0.37-0.95%). The quantity of sabinene and β-pinene were difference depended on cultivar of Citrus. The study of the effect on CNS in rats using the open field test demonstrated that the essential oil from som sai nam peung significantly exhibited CNS stimulant.

C5

C5_C0143 Chemical constituents from the twig of *Ziziphus attopoensis* Pierre.

Navarat Maneekaew[1], Piniti Ratananukul[1], Sunit Suksumrarn[1,*] and Apichart Suksumrarn[2]
[1]Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand
[2]Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand

Abstract: Five triterpenes, lupeol (**1**), betulinaldehyde (**2**), betulinic acid (**3**), alphitolic acid (**4**) and ursolic acid (**5**) together with one flavonoid, epicatechin (**6**) were isolated from the twig of *Ziziphus attopoensis* Pierre. The structures of all compounds were elucidated by analysis of their spectroscopic data and by comparision with the known compounds.

C5_C0149 An Automatic micro-sequential injection lab-on valve (μ-SI-LOV) coupled with PALM technology for determination of ranitidine

Jirayu Makchit[a], Boonsom Liawruangrath[a], Saisunee Liawruangrath[b,*]
[a] Applied Chemistry and Environment Research Unit, Institute for Science and Technology Research and Development, Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.
[b] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai 50200, Thailand.

Abstract: A miniaturized micro-sequential injection lab-on-valve (μSI-LOV) system coupled with PALM technology with spectrophotometric detection has been developed and evaluated. The PC of the μSI-LOV instrumentation can be substituted by a PALM computer with no differences in performance and sensitivity. Hardware and software (under PALM OS 3.5 and MS-Windows) are also developed by Hand-held Basic™ and MS-Visual Basic 6™. The resulting SI-LOV-PALM grams and the experimental data can be carried out by synchronization with PALM-Lab-Sync software. The proposed μSI-LOV-PALM spectrophotometric procedure has been applied for ranitidine determination in commercial pharmaceutical formulations. It is based on the reaction between tetrabromofluorescein and ranitidine in the presence of acid solution resulting in a pink, water soluble product with the absorption maximum at 545 nm. The software and the instrumentation as well as the simple and fully automation were demonstrated.

C5_C0174 Anti-HIV-1 RT Resistance Folds Prediction by AutoDock 3.0 and FRED Program

Sukhontip Thaomola, Chak Sangma
Cheminformatics Research Unit, Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok, Thailand.

Abstract: This study was aimed at using two docking programs, AutoDock and FRED, to predict the resistance folds of mutated HIV-RT over three anti-HIV drugs, nevirapine, AZT, and efavirenz. Staring with obtained complexes from molecular dynamics (MD) simulation of drug-enzyme which included 45 mutation types, AutoDock was used to reproduce the complexes. Then the AutoDock complexes were scored using various scoring functions in FRED in order to see if any of these scoring methods would result in good correlations with the MD simulations or experimental data. The results indicated that calculated scores were varied as the enzyme structures changed, however no correlations between the predicted resistance folds and the experimental data were found.

C5_C0194 Xanthones of mangosteen fruit with cytotoxicity activity against cancer cell lines

Orapin Komutiban[1], Piniti Ratananukul[2], Sunit Suksamrarn[2,*] and Apichart Suksamrarn[3]
[1] Program of Chemistry, Faculty of Science and technology, Suan Dusit Rajabhat University, Bangkok 10300, Thailand.
[2] Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand.
[3] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand.

Abstract: Three new xanthones, mangostenones C(1), D(2) and E(3), together with 16 known xanthones, were isolated from the young fruit of mangosteen (Garcinia mangostana). The structures of new compounds were elucidated by analysis of their spectroscopic data. Compound 1 showed cytotoxic properties against KB, BC-1 and NCI-H187 cancer cells with IC_{50} values of 2.8, 3.53 and 3.72 µg/ml, respectively. α- mangostin, the major metabolite, showed highest activity against BC-1 and KB cell at the respective IC_{50} values of 0.92 and 2.08 µg/ml, while gartanin displayed the activity against NCI -H187 cell at IC_{50} value of 1.08 µg/ml.

C5_C0198 Antiplasmodial and Antimycobacterial Activities of Triterpenes from the root barks of *Ziziphus cambodiana*

Panomwan Panseeta[1], Piniti Ratananukul[1], Thanomsin Distapom[1], Sunit Suksamrarn[1,*] and Apichart Suksamrarn[2]
[1] Department of Chemistry, Faculty of Science, Srinakharinwirot University, Bangkok 10110, Thailand.
[2] Department of Chemistry, Faculty of Science, Ramkhamhaeng University, Bangkok 10240, Thailand.

Abstract: 3-O-(4-hydroxy-3-methoxybenzoyl) ceanothic acid (**1**), a new ceanothane-type triterpene, was isolated from the root bark of *Z. cambodiana* (Rhamnaceae), together with eight known ceanothane- and lupane-type triterpenes, lupeol (**2**), betulinaldehyde (**3**), betulinic acid (**4**), 2-*O*-*E*-*p*-coumaroyl alphitolic acid (**5**), alphitolic acid (**6**), zizyberanalic acid (**7**), zizyberenalic acid (8) and ceanothic acid (9). The structure of all compounds were elucidated by analysis of their spectroscopic data. Compounds 1, 5 and 8 exhibited potent *in vitro* antiplasmodial activity against the parasite *Plasmodium falciparum* with IC_{50} values of 3.7, 0.9 and 3.0 µg/ml, respectively. Compounds 1 and 3-8 showed antimycobacterial activity against *Mycobacterium tuberculosis* with MIC values of 25, 25, 25, 12.5, 50, 50 and 100 µg/ml, respectively.

C5_C0273 SYNTHESIS OF NOVEL NAPHTHOQUINONE ESTER DERIVATIVES WITH ANTICANCER ACTIVITIES

Narathip Pradidphol[a], Boonsong Kongkathip[a], Komkrit Hasitapan[a], Pongpun Siripong[b], Jantana Yahuafai[b], Noojaree Prasitpan[a], and Ngampong Kongkathip[a]
[a] Natural Products and Organic Synthesis Research Unit (NPOS), Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand. [b] Natural Products Research Section, Research Division, National Cancer Institute, Bangkok, 10400, Thailand.

Abstract: Twelve novel naphthoquinone ester derivatives 9-20 were synthesized starting from 1-hydroxy-2-naphthoic acid (1). Benzoate esters 9, 10, 13, 14 and naphthoate esters 11, 12, 17, 18 were produced in 10 steps from 1 with high yield. Demethylation of 1-methoxy benzoate esters 13, 14 and 1-methoxy naphthoate esters 17, 18 using 1M boron tribromide in dichloromethane afforded 1-hydroxy benzoate esters 15, 16 and 1-hydroxy naphthoate esters 19, 20, respectively in 68-87 %yield. It was found that most of these naphthoquinone aryl esters exhibited moderate to strong anticancer activity against KB, HeLa, and $HepG_2$ cell lines.

C5_C0274 DETERMINATION OF AN ANTI-HIV-1 SUBSTANCE FROM *Clausena excavata*

Suriyan Sutthiprapar[1], Boonsong Kongkathip[1], Yupa Mongkolsook[2], Chalobon Yoosook[3] and Ngampong Kongkathip[1]
[1] Natural Products and Organic Synthesis Research Unit (NPOS), Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10903, Thailand.
[2] Kasetsart Agricultural and Agro-industrial Product Improvement Institute (KAPI), Kasetsart University, Bangkok 10903 Thailand.
[3] Department of Microbiology, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.

Abstract: *Clausena excavata* Burm f. (Rutaceae) is a shrub growing mainly in Thailand. It has medicinal properties such as treatment of snake-bite, antimalarial, anti-HIV-1 and pulmonary tuberculosis. There has been reported that five anti-HIV-1 constituents were isolated from *C. excavata*. Clausenidin is one of these constituents. This research discovered a new method for the determination of clausenidin from the crude extracts without isolation and purification. *C. excavata* was collected from ten provinces in Thailand which are Trad, Lampang, Chachoengsao, Chumporn, Sakonnakhon, Chiangmai, Chantaburi, Rayong, Kanchanaburi and Sisaket. The amounts of clausenidin in each crude ethanol extract, determined by HPLC analysis are different which were respectively, 0.063 0.054, 0.034, 0.025, 0.018, 0.013, 0.010 0.009, 0.008 and 0.000 % of dry weight.

C5_C0275 Extraction, isolation and antibacterial activity testing of Patchouli (*Pogostemon cablin*)

Pornpat Som-ang[(1)], Boonsong Kongkathip[(1)], Yupa Mongkolsook[(2)], Patcharee Sunthornanch[(3)] and Ngampong Kongkathip[(1)]
[(1)] Natural Products and Organic Synthesis Research Unit (NPOS), Department of Chemistry, Faculty of Science, Kasetsart University, Bangkok 10903, Thailand.
[(2)] Kasetsart Agricultural and Agro-industrial Product Improvement Institute (KAPI), Kasetsart University, Bangkok 10903 Thailand.
[(3)] Department of Microbiology , Faculty of Science, Kasetsart University , Bangkok 10903, Thailand.

Abstract: This research demonstrated two methods of extraction which are Soxhlet extraction with ethanol which gave crude ethanol extract in 15.98 % dry wt. and steam distillation after fermentation which yielded patchouli oil in 2.48 % dry wt. ,respectively. It was found that the crude ethanol extract contained patchouli oil and other highly polar constituents. Pure patchouli alcohol (patchoulol) was isolated from the crude ethanol extract by column chromatography (CC) in 0.58 %dry wt. and the structure was identified by spectroscopy. GC-MS analysis showed that patchouli alcohol is the main component in

the patchouli oil while the minor components are 4,7 – methanoazulene, *trans* - caryophyllene , alpha – guaiene, seychellene, azulene and pogostol. The antibacterial activity testing of the crude ethanol extract and the patchouli oil showed inhibition zones of *Staphylococcus aureus* and *Bacillus cereus*.

C5_C0276 DETERMINATION OF TETRACYCLINE RESIDUES IN MILK AND MILK PRODUCTS BY HIGH PERFORMANCE THIN LAYER CHROMATOGRAPHY

Boonsom Liawruangrath[1], Saisunee Liawruangrath[2], Wisanu Thongchai[1], Suwanna Saysin[1], Piyaporn Srisom[1], Jiraporn Chuangbunyat[1] and Theeraphan Machan[1]

[1] Department of Pharmaceutical Sciences, Faculty of Pharmacy, Chiang Mai University, Chiang Mai, 50200, Thailand.

[2] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai, 50200, Thailand.

E-mail: boonsom@pharmacy.cmu.ac.th

Abstract: A high performance thin layer chromatographic (HPTLC) method for determining tetracycline residues in milk and milk products was developed and validated. The samples were deproteinized and cleaned up. Then 10 µL of each sample solution was subjected to HPTLC analysis. The 10% citric acid : *n*-hexane : ethanol (80:1:1) solvent system was used for the quantitative evaluation of chromatograms. The peak area corresponding to the spot of tetracycline on the silica gel 60 G HPTLC plate (glass) was scanned in the reflectant/absorbance mode at 365 nm. Linear calibration curve was obtained over the range of 0.2 – 10.0 µg with r^2 = 0.9989. The limits of detection and quantitation were found to be 0.01 µg and 0.2 µg of tetracycline, respectively. The average recovery of the developed method was found to be 98.95% with the relative standard deviation of 1.44%. The proposed method has been applied to the determination of tetracycline residues in milk and milk products. Results are compared favorable with the AOAC Official Method.

D_D0001 PREPARE THE BISMUTH SILICATE ($Bi_{12}SiO_{20}$) POLYCRYSTAL FOR SINGLE CRYSTAL GROWTH

J. Kaewkhao[1*], J. Laopaiboon[2], R. Laopaiboon[2], S. Pencharee[2] and W. Chewpraditkul[3]
[1] Department of Physics, Nakorn Pathom Rajabhat University, Nakorn Pathom, 73000, Thailand
[2] Department of Physics, Ubon Rajathanee University, Ubon Rajathanee, 34190, Thailand
[3] Department of Physics, King Mongkut's University of Technology Thonburi, Bangkok, 10140, Thailand

Abstract: $Bi_{12}SiO_{20}$ polycrystalline material for the Bridgman-Stockbarger technique single crystal growth was prepared by solid state reaction, raw powder materials were mixed according to stoichiometry of Bi_2O_3:SiO_2 (non-crystalline) = 6:1 (mol%). X-ray diffraction (XRD) analysis and scanning electron microscope (SEM) were used to investigation on the sample. These results indicated that the sample is a single phase of $Bi_{12}SiO_{20}$ polycrystal, which can be used for single crystal growth.

D_D0002 Magnetoimpedance of cobalt-coated transformer cores

Somkane Piromrak, Pongsakorn Jantaratana and Chitnarong Sirisathitkul
Magnet Laboratory, Experimental Physics Research Unit, Institute of Science, Walailak University, 222 Thaiburi, Thasala District, Nakon Si Thammarat 80160, Thailand

Abstract: Magnetoimpedance (MI) of cobalt-coated silicon steels (1.28% Si) is studied. The samples, 0.4 x 0.5 x 55 mm were cut from sheets of transformer cores and coated with cobalt by electrodeposition. Composition, topography and magnetic properties of samples were analyzed. Magnetoimpedance was obtained by measuring electrical impedance (Z) of samples in applied magnetic field. The MI ratio ($\Delta Z/Z$) increased with frequencies, reached the maximum at the characteristic frequency and then decreased at frequencies above the characteristic value with increasing thickness of the cobalt layer, the MI ratio and the characteristic frequency decreased. The maximum 164 % MI ratio was observed at the characteristic frequency about 300 kHz for uncoated samples. Finally, MI ratio increased with increasing AC current from 1 to 20mA but this variation was modest in a high-frequency regime. The results can be explained by the dependence of the transverse permeability on the magnetic field, frequency and magnitude of AC current.

D_D0003 THERMAL CONDUCTIVITY OF GaAs/AlAs SUPERLATTICES USING 1D LINEAR-CHAIN MODEL.

กีรติ มณีสาย1, สมพร ขันเงิน1 และ ธนูสิทธิ์ บุรินทร์ประโคน1
1 ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ มหาวิทยาลัยขอนแก่น 40002
Email: or_pong@hotmail.com

Abstract: Thermal conductivity of GaAs/AlAs superlattices had been calculated from 1D linear-chain model phonon dispersion curve to investigate effect of structural parameters (ie. thickness of symmetric and anti-symmetric structures) to superlattices phonon dispersion relation, density of states, group velocity and thermal conductivity along cross-plan direction. The results show that there are some differences between GaAs/AlAs superlattice phonon dispersion relation and their bulk dispersion which modify density of states, group velocity and reduce superlattice longitudinal thermal couductivity.

D_D0004 SIMULATION OF THE MOTION OF A BODY UNDER THE EARTH 'S GRAVITATIONAL FORCE.

Chanruangrit Channok
Department of Physics, Faculty of Science, Ubonratchathani University, Ubonratchathani, 34190 Thailand.
E-mail: physics007@yahoo.com, Fax: (664)-528-8381

Abstract: We simulated the motion of a body fall to the Earth under the Earth's gravitation. In real physical phenomenon, the form of ordinary differential equation for equation of motion is non-linear, $\ddot{x} = GM / x^2$ This equation cannot be solved by an analytical method. We used a computational method to solve problem by apply the 4th order Runge-Kutta Method. We found that simulation results are different from calculation in a linear case about ± 5.8 %, when the body fall to Earth's ground at distance over 500 kilometer.

D_D0005 STRUCTURAL AND OPTICAL CHARACTERIZATION OF SODIUM DOPED $CuInSe_2$ THIN FILMS GROWN BY THERMAL EVAPORATION METHOD

Ngamnit Wongcharoen, Thitinai Gaewdang, Pakorn Sittiketkorn*, Thitikorn Chanyatham and Prathan Prachopchok.
Department of Applied Physics, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Chalongkrung Rd., Ladkrabang, Bangkok 10520, Thailand;
*Corresponding author, E-mail ; pakorn_s1@hotmail.com

Abstract: Na-doped $CuInSe_2$ (CIS) thin films were prepared by using sodium compounds such as Na_2S and $Na_2S_2O_3$ on glass slide substrate. The samples have been deposited in a two-stage process. In the first stage, the precursors were evaporated on glass substrate by thermal evaporation method in vacuum chamber. The selenization, named the second stage, was performed inside a partially closed graphite box. The last one was realized at 550 °C for 30 min in argon atmosphere with elemental selenium incorporation. The obtained polycrystalline Na-doped CIS films showed the chalcopyrite structure with predominant growth in the (112) orientation. The structural parameters such as lattice constants and crystallize size have been evaluated. The energy gap values were 0.96, 1.16, 1.19 eV for non-doped, Na_2S and $Na_2S_2O_3$ doped CIS film respectively.

D_D0006 PATTERNED-SUBSTRATE GROWTH BY BALLISTIC DEPOSITION MODEL WITH THERMAL ACTIVATION

Chalasai Chaiyasorn, and Patcha Chatraphorn
Department of Physics, Faculty of Science, Chulalongkorn University, Phayathai Road, Pathumwan, Bangkok 10330, Thailand.
E-mail: chalamay@yahoo.com

Abstract: When creating nanoscale devices, it is very important that atomic arrangement can be controlled. In this study, ballistic deposition model with thermal activation is selected as a tool. The goal is to determine conditions that will help in maintaining a pattern on the substrate throughout the growth process. Two types of pattern, flat and periodic patterns, are used. Persistence probability is calculated to see how much the pattern still remains at a specific time. Simulation results show that the persistence probability in both systems decreases with time. If the time is fixed, the substrate temperature plays an important role with the persistence probability peaking at approximately 700 K. It is also found that the persistence probability in the periodic patterned substrate system is smaller than that in the flat pattern system.

D_D0007 THE DISTRIBUTION AND VARIATION OF GROUND TEMPERATURE UNDER NATURAL CLIMATIC CONDITIONS OF PHATTHALUNG PROVINCE

Nant Klonpong[1,*] J. Waewsak[2] M. Mani[2] and S. Phethuayluk[2]
[1] Graduate Student, B.Sc. (Physics), Physics Department, Faculty of Science, Thaksin University, Songkhla, 90000, Thailand
[2] Renewable Energy System Research and Demonstration Center (RERD) Physics Department, Faculty of Science, Thaksin University, Phatthalung, 93110, Thailand
E-mail address: klompong_rit@hotmail.com

Abstract: This research aims is to investigate the distribution and variation of temperature in ground under natural climatic conditions of Phatthalung province in order to study the feasibility of the utilization of ground as heat sink in refrigerating system for increasing the C.O.P. of the system. Experiments were set up by measuring ground temperature at surface, 0.5 1.0 1.5 2.0 2.5 and 3.0 m depth. Solar radiation intensity, ambient air temperature and humidity including speed and direction of wind were also measured for developing mathematical model to describe the behavior of distribution and variation of ground temperature. Results showed that ground surface temperature varied depending on the intensity of solar radiation. The maximum and minimum ground surface temperature were about 35 °C (2 p.m.) and 25 °C (5 a.m.). The ground temperature varied slightly a depth of 1.5 – 2 m. Furthermore, the 2 m depth was the suitable depth for applying as heat sink due to the ground temperature was lower than that of 1 m and 3 m during daytime.

D_D0008 THE STUDY OF MAGNETIC FIELD OVER A MAGLEV'S RAIL MODEL

Piti Panichayunon, Chat Pholnak, Supagone Katatikarnkul, Rungdaow Dumsri
Department of Physics, Faculty of Science, Thaksin University, Songkla,Thailand.
E-mail:piti204@yahoo.com, Tel: (074) 693995, Fax : (074) 693995

Abstract: The Magnetically levitated (Maglev) train is a new interesting alternative transportation which gives super-high-speed running and the low environmental impact. Maglev train has such high speed because it has no contact with rail. The magnetic force contributes the levitation while the linear motor technology causes the forward motion. From the result, we found that the increase of the applied current leads to the increase of the magnetic field that mean the increase of the levitation force. Moreover the magnetic field over its rail is Gaussian distribution which has a maximum value at the middle of the solenoid. Overall intensity of the magnetic field tends to decrease as a function of distance away from the current source. This gradient of the magnetic field causes of the forward motion of the Maglev train.

D_D0009 PERIOD CHANGE IN A δ SCUTI VARIABLE AD CANIS MINORIS

Wiraporn Maithong[1], Amnart Sukom[2]
[1] Faculty of Science and Technology, Chiang Mai Rajabhat University, Chiang Mai 50300, Thailand
[2] Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand

Abstract: Period change analysis, using the IRAF technique, in order to determine the photometry, the pulsing period and the period change of a variable star. AD Canis Minoris is a δ scuti variable star having a pulsing period of 0.12297 day. The O-C analysis shows an increase of the orbital period which means that the star might be going to the post main sequence. A periodic shape evaluated from the residual may also suggest the presence of a binary system, having the period of 26.94 years and the orbital radius of 0.5322 AU.

D_D0010 TRAPPING AND DIFFUSIVE ESCAPE OF FIELD LINES IN TWO-COMPONENT MAGNETIC TURBULENCE

Piyanate Chuychai[1], David Ruffolo[2], William H. Matthaeus[1], and Jakrapan Meechai[3]
[1] Bartol Research Institute, University of Delaware, Newark, DE 19716, USA.
[2] Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand,
e-mail: david_ruffolo@yahoo.com, FAX: (662)-201-5762.
[3] Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

Abstract: Recent studies have shown that transport along magnetic field lines admits a surprising degree of persistent trapping due to small-scale topological structures (1-2). This underlies the partial filamentation of magnetic connection from small regions of the solar corona to Earth orbit, as indicated by the observed dropouts (inhomogeneity and sharp gradients) of solar energetic particles. We explain this using a two-component model with slab and two-dimensional (2D) fluctuations, which has provided a useful description of solar wind phenomena. We present an analytic theory, confirmed by simulations, for the trapping length and its dependence on various parameters. We provide a quasilinear theory, again confirmed by simulations, for the suppression of field line diffusion. We find that the filamentation of magnetic connectivity to the source is sharply delineated by local trapping boundaries, defined as local maxima in the mean squared field along the 2D orbit, because of the suppression effect.

D_D0011 DESIGN AND CONSTRUCTION OF A DEVICE FOR MEASURING ROTATIONAL MOTION.

Supphadate Sujinnapram[1], Bancha Silskulsuk[1], and Nason Phonphok[1]
[1] Department of Physics, Faculty of Science, Srinakharinwirot University, Sukhumvit 23, Bangkok 10110.
E-mail address: supphadate@yahoo.com

Abstract: An electronic angular measuring instrument which angular displacement can be measured via a circular scaled on transparency film was made. The device can be used to measure angular instantaneous motions by interfacing with computer parallel port controlled by a home-made program. Relationships of angle, angular speed, distance and speed with respect to time, can be displayed promptly on a monitor and recorded as computer text files. Accuracy tests were done in terms of the Earth's gravitational acceleration obtained by an Atwood's machine. The gravitational acceleration value of 9.77 m/s^2 was obtained which is 0.1% deviated from the value provided by the National Institute of Metrology (Thailand).

D_D0012 A study order of acoustic mode for type of gas analysis

Padung Laeyadsintapa, Sorasak Danworaphong
Experimental Physics Research Unit, School of Science, Walailak University, Nakhon Sri Thammarat, Thailand

Abstract: The fundamental mode of acoustic resonance in a tube can be used to determine the sound speed and the molecular mass of a pure sample gas. When the sound speed and molecular mass of two gases are closed, only the fundamental mode determination becomes inadequate due to the peak overlapping. In this work, the resonance frequency is used to calculate the sound speed from which it relates to the molecular mass of the sample gas and studies have been done at the 7th harmonic for different standard gases and the resolution of the designed system is obtained to be 1.63 Hz for the change in velocity of 1 m/s. The higher harmonic the better resolution. However, the tradeoff is the decrease in acoustic amplitude. The system is designed for open-air measurement applications.

D_D0013 PRECIPITABLE WATER VAPOR METER

Sayan Phokate[1], Jongruk Samart[2], Panich Kanchai[1], Wimonrut Thongphuton[1] and Apiwat Boonkhuang[1]
[1] Division of Science, Khon Kaen Campus, Rajamangala University of Technology Isan 40000, Thailand, syphokate@hotmail.com
[2] Division of Electronic, Khon Kaen Campus, Rajamangala University of Technology Isan 40000, Thailand.

Abstract: In this research, the researcher has built the precipitable water vapor meter. The meter was built relying on the relative humidity data and the temperature acquired from the upper air data in coherence with the relative humidity and the temperature acquired from the surface data in the same meteorological station in a form of a mathematics model. The model was then used to create the meter by connecting the relatively humidity and temperature sensor to the micro controller. The meter would read the precipitable water vapor value in centimeters. When the meter was completed, it was used to collect the data from the meteorological station to compare with the precipitable water vapor value acquired from the same station at the upper air checking data. The data showed that the water vapor value acquired through the meter with the R-squared of 0.90.

D_D0014 TITANIUM DIOXIDE THIN FILMS PREPARED BY ION-ASSISTED E-BEAM EVAPORAION FOR GAS SENSING APPLICATIONS

C. Promjantuk[1], A.Wisitsoraat[2] and P. Limsuwan[1]
[1] Department of Physics, King Mongkut's University of Technology Thonburi (KMUTT), 91 Prachautit Rd. Thungkru, Bangmod, Bangkok, 10140 Thailand.
Email: opticslaser@yahoo.com,TEL:02-470-8868,02-872-5253,FAX:02-872-5254
[2] Nanoelectronics and MEMS Laboratory, National Electronics and Computer Technology Center,112 Thailand Science Park, Pahol Yothin Rd., Klong Laung, Pathumthani 12120,Thailand.

Abstract: TiO_2 is promising gas-sensing material due to its high temperature stability and catalytic properties. The physical and gas-sensing properties of the TiO_2 gas sensor depend on the method and the condition of film preparation. In this work, we study the gas sensing behaviour of TiO_2 thin film prepared by electron beam evaporation with ion-assisted deposition (IAD). TiO_2 thin film has been characterized for structural and gas-sensing characteristics as a function of IAD deposition parameters, including ion power and oxygen flow rate and pressure, with the film thickness in nanometer scale. From structural characterization by X-ray diffraction (XRD) and scanning electron microscope (SEM), the as-deposited TiO_2 thin film has amorphous structure with smooth surface. After annealing at 400 °C, the TiO_2 film becomes polycrystalline structure with

sub-micrometer grain size and anatase phase with (101) preferred orientation. The sensors were tested with different gases, including ethanol and acetone. The experimental results show that 30 nm-thick TiO_2 thin films exhibit high sensitivity to low concentration acetone and ethanol in the range of 100 ppm with optimum operating temperature about 400 °C.

D_D0015 AEROSOL ANALYSIS IN CHAING MAI PROVINCE BY PROTON INDUCED X-RAY EMISSION (PIXE) TECHNIQUE

ช่ออัญชัน ประพันธ์ศรี[1], ธีรศักดิ์ คำวรรณะ[2], โฉม ทองเหลื่อม[1], สมศร สิงขรัตน์[2]
[1]สถาบันวิจัยและพัฒนาวิทยาศาสตร์และเทคโนโลยี มหาวิทยาลัยเชียงใหม่
[2]ภาควิชาฟิสิกส์ คณะวิทยาศาสตร์ มหาวิทยาลัยเชียงใหม่

Abstract: Particulate pollution is considered a cause of adverse health effects. The Pollution Control Department, Ministry of Natural Resources and Environment, has 2 air pollution inspection sites in Chiang Mai. The Yupparaj School site is located in an urban area. The government center (City Hall) site is located in a rural area. The aerosol samplers are air monitoring type EC9800 ambient air analyzers. The aerosol filters are Teflon with 47 millimeter diameter and 5 micrometer pore size. Replacement of aerosol filters is performed every 2 weeks. We temporarily analyze the above mentioned filters by Proton induced X-ray emission (PIXE) technique. The results are used to infer the elemental composition of the aerosol. PIXE is one of the efficient, non-invasive analysis techniques. Advantages of the PIXE technique are the capability to analyze quantitatively in parts per million (ppm), a fast analysis and high sensitivity. PIXE technique is used with a 1.7 MV tandem "Tandetron" accelerator at Chiang Mai University. Hydrogen plasma is produced by Duoplasmatron source. Hydrogen ions (H^+) or protons are accelerated in the accelerating tube to obtain energy of 2 MeV. Very low current about 0.1 nA is used in PIXE analysis. The characteristic X-ray produced from the aerosol sample is detected by the Si(Li) detector Model SSL30150. Quantitative analysis provided the different amounts of elements, such as Al, Si, S, Cl, K, Cr and Fe, at various times. The standard program, GUPIX, is used for quantitative analysis. It found that the amounts of detected elements are in the range of 1658 -152, 912 ppm. Sulphur (S) is still observed at some times but the heavy metal elements such as Pb and Hg, which are health hazards, are not observed in the aerosol of Chiang Mai.

D_D0016 COMPARISON OF STRUTURAL PROPERTIES OF LINEAR GRADED AND STRAIN-LAYER SUPERLATTICE InGaAs BUFFER LAYERS

Pornsiri Konglaeng[1], Sakuntam Sanorpim[1], and Kentaro Onabe[2]
[1] Department of Physics, Faculty of Science, Chulalongkorn University, Pathumwan, Bangkok 10330, Thailand
` E-mail: Pornsiri.Ko@student.chula.ac.th, Tel : (662) 218- 7689, Fax : (662) 253-1150
[2] Department of Advanced Materials Science, The University of Tokyo, Japan

Abstract: In this work, we investigated structural properties of the linearly-graded (LG) and strained-layer superlattice (SLS) InGaAs buffer layers grown on GaAs substrates by metalorganic vapor phase epitaxy (MOVPE). Our results show that the generation of dislocations (misfit and threading dislocations) investigated by cross-sectional transmission electron microscopy (TEM) was found to be dominated in the LG-InGaAs regions. This means that the LG-InGaAs buffer layer was relaxed due to the large lattice-mismatch between InGaAs and GaAs, resulting in generation of a large number of dislocations. On the other hand, for the SLS-InGaAs buffer layer, a high density of dislocations was observed in the InGaAs/GaAs superlattice regions. In fact, density of dislocations decreased in the InGaAs top layer grown on the InGaAs/GaAs superlattice. This demonstrates that the strained-layer superlattice exhibits some filtering of threading dislocations. Also, the strain-relaxation will be discussed in comparison between LG- and SLS-InGaAs buffer layers.

D-D0017 DETERMINATION OF NITROGEN CONCENTRATION IN GaAsN FILM BY RAMAN SCATTERING

Panatda Panpech[1], Sathon Vijarnwannaluk[1], Sakuntam. Sanorpim[1], Wataru Ono[2], Fumio Nakajima[2], Ryuji Katayama[2] and Kentaro Onabe[2]
[1] Department of Physics, Faculty of Science, Chulalongkorn University, Phayathai Rd., Pathumwan, Bangkok 10330, Thailand; E-mail: Panatda.P@Student.chula.ac.th, Tel: 218-7529
[2] Department of Advanced Materials Science, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8561, Japan;

Abstract: Raman scattering were used to study $GaAs_{1-x}N_x$ alloy films ($0 \le x \le 0.055$) grown on GaAs (001) substrates by metalorganic vapor phase epitaxy (MOVPE). In the N-incorporating films, a single N-related local vibrational mode (LVM) is observed at around 468 - 475 cm^{-1}. We have investigated the integrated intensity (I_{LVM}) and frequency (ω_{LVM}) of the N-related LVM as a function of N concentrations. It is evident that both I_{LVM} and ω_{LVM} increase with increasing N concentrations. The N concentrations in the films determined by Raman spectroscopy technique (x_{Raman}) exhibits a linear dependence on the N concentrations determined by the high resolution X-ray diffraction (HRXRD) (x_{XRD}). Our results demonstrate the linear dependence of the x_{Raman} on the x_{XRD}, which provides a useful calibration method to determine the N concentrations in dilute $GaAs_{1-x}N_x$ films ($x_{XRD} \le 0.055$). In addition, a reduction of bandgap with higher N incorporation was clearly observed by photoluminescence (PL) spectra. A correlation between the bandgap reduction and the examined N concentration was analyzed.

D_D0018 RED EMISSION FROM InGaPN/GaP LATTICE-MATCHED SINGLE QUANTUM WELL STRUCTURES GROWN BY MOVPE

Dares Kaewket[1*], Sukkaneste Tungasmita[1], Sakuntam Sanorpim[1], Fumihiro Nakajima[2], Nobuhiro Nakadan[2], Tokuharu Kimura[2], Ryuji Katayama[2] and Kentaro Onabe[2]

[1] Department of Physics, Faculty of Science, Chulalongkorn University, Phayathai Rd., Pathumwan, Bangkok 10330, Thailand.

[*] E-mail: Dares.K@Student.chula.ac.th, Tel: (662)218-7689, Fax: (662)253-1150

[2] Department of Advanced Materials Science, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8561, Japan.

Abstract: In this study, optical properties of $In_xGa_{1-x}P_{1-y}N_y/GaP$ lattice-matched single quantum wells (SQWs) grown on GaP (001) substrates by metalorganic vapor phase epitaxy (MOVPE) with various well widths (L_z = 1.6-6.4 nm) and different In (x = 0.056, 0.108, 0.176) and N (y = 0.025, 0.048, 0.071) concentrations have been investigated by using low-temperature photoluminescence (PL) and PL excitation (PLE). The PL spectra showed the strong red emission from the samples which attracted to apply using in a variety of optoelectronic device applications such as light emitting and laser diodes. Comparing to the bulk film, the PL peak position and the fundamental absorption edge of PLE spectra exhibit blue-shift, which are believed to be principally determined by the quantum confinement effect to the well. With an increasing N concentration, the PL peak and absorption edge exhibit red-shift due to the lowering conduction band edge. On the other hand, PL intensity significantly decreases for the SQWs with higher N concentrations. This probably caused by the dominantly non-radiative process which related to N-induced trap states.

D_D0019 THERMAL ANNEALING EFFECT ON THE OPTICAL PROPERTIES OF $GaAs_{1-x}N_x$/GaAs MULTIPLE QUANTUM WELLS STRUCTURE WITH HIGH N CONTENT GROWN BY MOVPE

Pawinee Klangtakai[1], Sakuntam Sanorpim[1], Kajornyod Yoodee[1], Wataru Ono[2], Fumio Nakajima[2], Ryuji Katayama[2] and Kentaro Onabe[2]

[1] Department of Physics, Faculty of Science, Chulalongkorn University, Phayathai Road, Pathumwan, Bangkok 10330, Thailand. E-mail: Pawinee.K@student.chula.ac.th, Fax: (662) 253-1150.

[2] Department of Advanced Materials Science, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8561, Japan.

Abstract: Effects of thermal annealing on optical properties of $GaAs_{0.949}N_{0.051}$/GaAs multiple quantum wells (MQWs) grown on GaAs (001) substrate by metalorganic vapor phase epitaxy (MOVPE) were investigated. Photoluminescence (PL) results of as-grown sample show an electron confinement in the $GaAs_{0.949}N_{0.051}$/GaAs MQWs. After thermal annealing, blue-shift of the PL peak energy was clearly observed. Thermal annealing induces diffusion of N out of the quantum well and homogenizes the N distribution fluctuations. According to x-ray diffraction (XRD) analysis, the blue-shift in the PL can in part be attributed to reduction in N concentration in side the well. The more homogeneous N distribution leads to a reduction in full width at half maximum of PL spectra. In addition, both the as-grown and annealed $GaAs_{0.949}N_{0.051}$/GaAs MQWs samples, which were characterized by XRD and transmission electron microscope (TEM), exhibit a fairly flat and abrupt $GaAs_{0.949}N_{0.051}$/GaAs interfaces.

D_D0020 ^{40}K, ^{226}RA AND ^{232}TH ANALYSIS IN SONGKHLA BEACH SANDS USING GAMMA RAY SPECTROMETRY

Prasong Kessaratikoon[1], Supawut Benjakul[2], Suchin Udomsomporn[3]

[1,2] Department of Physics, Faculty of Science, Thaksin University, Songkhla 90000, Thailand.

[3] Bureau of Technical Support for Safety Regulation, Office of Atoms for Peace, Bangkok 10900, Thailand.

Abstract: The activity concentrations and the gamma-absorbed dose rates of the terrestrial occurring radionuclides viz. ^{40}K, ^{226}Ra and ^{232}Th were determined in 80 beach sands samples collected along the Chalatat and the Samila beaches in Songkhla province, using gamma ray spectrometry. The beach sand activity ranges from 89.15 – 963.54 Bqkg^{-1} for ^{40}K, 0.00 - 120.03 *Bqkg*$^{-1}$ for ^{226}Ra and 0.00 – 318.79 *Bqkg*$^{-1}$for ^{232}Th with mean values of 247.88 *Bqkg*$^{-1}$, 23.56 *Bqkg*$^{-1}$ and 63.88 *Bqkg*$^{-1}$, respectively. The activity concentration of these radionuclides are compared with the OAP results and other global radioactivity measurements and evaluations. Radium equivalent activities are calculated for the analyzed samples to assess the radiation hazards arising. All the beach sands samples have radium equivalent activities lower than the limit set in the OECD report (370 *Bqkg*$^{-1}$).

D_D0021 NATURAL RADIONUCLIDE DISTRIBUTION IN SOIL FROM MUANG DISIRICT IN SONGKHLA PROVINCE

Supphawut Benjakul[1], Prasong Kessaratikoon[2], Suchin Udomsomporn[3]

[1,2] Department of Physics, Faculty of Science, Thaksin University, Songkhla 90000, Thailand.

[3] Bureau of Technical Support for Safety Regulation, Office of Atoms for Peace, Bangkok 10900, Thailand.

Abstract: The concentrations of primordial radionuclides in 40 soil samples collected from Muang district in Songkhla province has been measured from the gamma ray spectrum of the soil. The mean activities of ^{40}K, ^{226}Ra and ^{232}Th are found to be 1029.36 *Bqkg*$^{-1}$, 68.41 *Bqkg*$^{-1}$and 96.48 *Bqkg*$^{-1}$ dry weight, respectively. The average outdoor absorbed dose rate in air at a height of 1 m above ground is 139.81*nGyh*$^{-1}$, corresponding to an annual effective dose equivalent of 857.31 μSv. The results have been compared with other global radioactivity measurements and evaluations.

D_D0022 COMPARISON OF CsI(Na) AND BGO SCINTILLATORS IN GAMMA-RAY SPECTROMETRY

Chalerm Wanarak[1], Weerapong Chewpraditkul[2,*], Panutut Boonpramuk[1]

[1] Industrial Metrology Program, Faculty of Engineering King Mongkut's University of Technology Thonbubi, Bangkok 10140, Thailand

[2] Radiation Physics Laboratory, Department of Physics, Faculty of Science King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand

Abstract: The scintillation response of CsI(Na) and BGO scintillators have been compared using photomultiplier tube readout for photon energies ranging from 31 keV to 1274 keV. The energy resolution (FWHM), obtained in this work, for 662 keV γ-rays from ^{137}Cs, are 8.6% and 14.7%, respectively, for CsI(Na) and BGO. The study showed that the light yield of CsI(Na) is superior above BGO, while its photofraction is inferior to that of BGO. Both crystals showed a light yield nonproportionality relative to the yield at 662 keV γ-peak, especially in the energy region below 356 keV.

D_D0023 THE BEHAVIOR OF A DRIPPING WATER FROM A FAUCET

Uraiwan Petlum[1], Panatcha Anusasananan[2] Damrongsak Maneepongswadi[3], Nipon Thangprasert[4]

[1,2,3,4]Department of Physics, Faculty of Science, Ramkhamhaeng University, Bangkok 10240;

e-mail address : nipon@ram1.ru.ac.th

Abstract: In this research we study the characteristics of water dripping when the rate of flow changes. With a slow rate of flow, the periodic dripping was found in the following types: 1T, 2T and 4T. With an increased rate of flow, the results indicated motion of the chaotic type, which was the main characteristic of non-linear system. When we carefully investigate the chaotic region, we can observe a structure in it. It is not completely random but some points are constrained within a finite shape. This is another view of the strange attractor.

D_D0024 COMPOSING MUSIC USING THE FRACTAL TREES

Damrongsak Maneepongswadi [1], Panatcha Anusasananan[2],Chom Sosawang[3], Nipon Thangprasert[4]

[1,2,4]Department of Physics, Faculty of Science, Ramkhamhaeng University, Bangkok 10240;

e-mail address: nipon@ram1.ru.ac.th

[3] Sirirattanathom school, Udomsouk 30, sukhumvit 103, Bangna, Bangkok 10260.

Abstract: Music and physics always has a close relationship. Chaos, fractals and self-similarity are tropics which caught public interest. Fractals are geometric object that have many application in science. Their structure can be used to model computer generation of images that may be visually very attractive. Many relations have been discovered in recent years between fractals and music. In this research we create music from fractals using the same types of iterative processes used to create fractal images with the help of a few computer program. We use only one instrument, 73 flute, to play this song in order to analyze the spectrum of the song and study the symmetry that actually forms the background of the self-similarity in the song. Then we add the MIDI drum to the song to make it more enjoyable. After having several person listen to the song, 70% satisfy with this song. We can compose the song using the fractal trees since their structures are not completely random but have some pattern the same way that the music consists of a set of notes which usually exhibit similarity sequences of some group of notes.

D_D0025 Physical Properties of Bulrush Culms (Lepironia articulata) in Raw Material Preparing Process of Talaenoi Community

Chat Pholnak[1], Suwit Pechhuayluk[1], Pompana Buapech[1] and Piti Panichayunon[1]

[1] Renewable Energy System Research and Demonstration Center, Department of Physics, Faculty of Science, Thaksin University, Phatthalung 93110, Thailand;

E-mail address: chat432@hotmail.com

Abstract: In this research, we emphasize to study the physical properties of bulrush culms (Lepironia articulata) which is a raw material in weavings product of Talaenoi community. Such properties are shape, moisture and strength. It was found that all bulrush culms had decreased size fractal with its length, in position of bottom, middle and top of culms were about 5.25±0.76 mm, 4.38±0.53 mm and 3.50±0.34 mm, respectively. The thicknesses were about 0.66±0.14 mm, 0.69±0.08 mm and 0.55±0.05 mm, respectively. The initial and final moisture content of green and dry bulrush culms were investigated based upon AOAC standard and found to be 87.56% and 16.11%, respectively. Finally, the result of strength by tensile force was about 82.00±20.07 N.

D_D0026 Anisotropy signatures of solar energetic particle transport in a closed interplanetary magnetic loop

ALEJANDRO SÁIZ[1], DAVID RUFFOLO[1], JOHN W. BIEBER[2], PAUL EVENSON[2], AND ROGER PYLE[2]

[1] DEPARTMENT OF PHYSICS, MAHIDOL UNIVERSITY, BANGKOK, THAILAND

[2] BARTOL RESEARCH INSTITUTE, UNIVERSITY OF DELAWARE, NEWARK, DELAWARE, USA

Abstract: When solar energetic particles travel along a closed interplanetary magnetic loop produced by a previous solar event, there exists the possibility that they arrive along the longer leg of the loop from the Sun to the place of their detection, instead of the short leg, so they are first detected moving sunwards. We use state-of-the-art numerical simulations of solar energetic particle transport to show that, in such case, the measured distribution of particles cannot have arbitrarily

large anisotropy because of mirroring effects, and we conclude that the described scenario cannot be used to explain the observations during the October 28, 2003 ground level enhancement of cosmic rays.

D_D0027 PARTICLE TRAPPING IN 2D + SLAB MAGNETIC TURBULENCE IN A SPHERICAL GEOMETRY

Paisan Tooprakai[1,2,3], David Ruffolo[2], William H. Matthaeus[3], and Piyanate Chuychai[3]
[1] Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.
[2] Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand .
[3] Bartol Research Institute, University of Delaware, Newark, DE 19716, USA.

Abstract: An impulsive solar flare event was measured by the ACE spacecraft, with rapid changes in the intensity of the solar energetic particles (SEPs) in which the intensity appears and disappear repeatedly, called "dropouts." This indicates filamentation of the particle distribution, and several astrophysics groups have tried to explain these events using computer simulations. We evaluate the particle trajectories in the slab + 2D magnetic fields using the fundamental Newton-Lorentz equations in spherical coordinates. We simulate the motion of charged particles at different energy levels in the same magnetic field, which shows that the low energy particles closely follow the slab + 2D magnetic fields, showing dropout features, but these are washed out for high energy particles at about 1 AU.

D_D0028 TRAPPING OF MAGNETIC FIELD LINES IN ISLANDS OF TURBULENCE.

Nimit Kimpraphan[1,2], David Ruffolo[2], and Soliphong Chatraphorn[1]
[1] Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand, e-mail: mit@astro.phys.sc.chula.ac.th, FAX: (662)-201-5762.
[2] Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.

Abstract: The two-component model of magnetic turbulence, including the slab and the two-dimensional components following (1), can successfully explain the dropout phenomena of solar energetic particles. We can consider that the solar energetic particles follow the magnetic field lines from the Sun. These magnetic field lines are trapped in the small-scale structures called the "magnetic islands" for a while before diffusing throughout all space. Simulation methods, e.g., the Box-Counting Method, the Anisotropy Method, the Dual Lattice Method, and the Principal Component Method, are developed and used to analyze the data from tracing the magnetic field lines in turbulent fields. We vary the magnetic parameter values, e.g., the fluctuation energy to the mean field energy ratio, the radius of the initial circle, the parallel length scale, and the perpendicular length scale. From the analysis results, we can obtain conditions and length scales over which dropouts can occur.

D_D0029 MAGNETIC FIELD LINE RANDOM WALK IN ISOTROPIC AND SPHEROIDAL TURBULENCE

Pat Wongpan[1], David Ruffolo[1], William H. Matthaeus[2], and George Rowlands[3]
[1] Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand,
e-mail: pattyphys@yahoo.com, FAX: (662)-201-5762.
[2] Bartol Research Institute, University of Delaware, Newark, DE 19716, USA.
[3] Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Abstract: Many types of space and laboratory plasmas involve turbulent fluctuations with a mean magnetic field B_0, and the field line random walk plays an important role in guiding particle motions. The 2 coupled integral equations for field line diffusion coefficients $D_x = D_y$ and D_z, with D dependence inside 3-dimensional integrals over k-space, are solved numerically to verify our analytic results. Our results indicate that the field line random walk is always close to isotropic, within a factor of 2, even for very anisotropic turbulence. For a given power spectrum, we find quasilinear behavior at high B_0 and percolative behavior at low B_0. We provide closed-form solutions at high B_0 and for isotropic, very prolate, or very oblate turbulence at low B_0.

D_D0030 ELECTRONIC STRUCTURES OF Bi_2Te_3 CALCULATED BY DV-Xα METHOD

Thaweewat Khuangthip, Tosawat Seetawan
Physics Program, Faculty of Science and Technology, Rajabhat Sakon Nakhon University, 680 Nittayo Road, Sakon Nakhon, Thailand.
E-mail:khuangthip@yahoo.com, Fax: (664)271-3812

Abstract: Electronic structures of bismuth telluride (Bi_2Te_3) calculated by DV-Xα method it compose of model cluster, energy level and density of state.The cluster model of Bi_2Te_3 using the group number was 166 (p3m) and cell parameters a=b=c was 10.45 and α=24.13. Electron configuration of Bi_2Te_3 separated Bi: 1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p and Te: 1s 2s 2p 3s 3p 4s 3d 4p.Energy level showed conduction band about 2.5 eV and valence band of electrons in atom about -2.5. Density of state showed high in negative level that means p-type conductivity was confirmed this experiment.

D_D0031 The Distribution Analysis of the Solar Energetic Particle in Various Directions

Sugunya Mongkol, Thiranee Khumlumlert
Department of Physics, Faculty of Science, Naresuan University, Phitsanulok, Thailand
*corresponding autor: thiraneek@nu.ac.th

Abstract: We analyze the distribution of solar energetic particle (SEP) data collected from STEP/WIND (The Suprathermal Energetic Particle System/WIND Spacecraft) of 2 solar events , which are on September 7 , 2005 (the normal solar wind speed of 390 km/s) and January 20 , 2005 (the high solar wind speed of 822 km/s) . When we use IDL (Interactive Data Language) program to analyze the SEP propagate through the interplanetary medium in different direction for spacecraft and solar wind frame , then we found that the solar wind speed affected to the distribution of particle in various direction. The solar event with the high solar wind speed in solar wind frame found the inward and outward particle distribution along the magnetic field line from the Sun, but we found the less effect of different distribution of SEP with the normal solar wind speed for the both frames.

D_D0032 The Solar Energetic Particle Propagation

Nikorn Panrun, Thiranee Khumlumlert
Department of Physics, Faculty of Science, Naresuan University, Phitsanulok, Thailand
*corresponding autor: thiraneek@nu.ac.th

Abstract: We simulate the propagation of solar energetic particle released from the Sun by the transport equation of Ruffolo (1998) with the numerical method, and we analyze the distribution profile of particle with IDL (Interaction Data Language) and Origin7 for the solar event on September 7,2005. We compare the simulation results with the read data from SIS/ACE (Solar Isotopic Spectrometer/Advanced Composition Explorer Spacecraft). We find the dense pulses of particle rapidly propagate outward in the strong focusing region near the Sun, then they slowly decay and more diffusion with increasing distance from the Sun. We found trend of the mean free path increase as energy and the range of propagation distance along the magnetic field line is 0.65 AU to 1.35 AU.

D_D0033 EFFECT OF BORON DOPANT ON THE PROPERTIES OF $Cd_{0.6}Zn_{0.4}S$ THIN FILMS PREPARED BY THERMAL EVAPORATION

Thitinai Gaewdang, Ngamnit Wongcharoen, Thitikorn Chanyatham*, Pakorn Sittiketkorn, Nathaporn Promros and Prathan Prachopchok
Department of Applied Physics, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Chalongkrung Rd., Ladkrabang, Bangkok 10520, Thailand;
*Corresponding author, E-mail: thitikorn_c@hotmail.com

Abstract: Boron doped $Cd_{0.6}Zn_{0.4}S$ thin films were deposited on glass substrates by thermal evaporation from mixed CdS and ZnS compounds using B_2O_3 as a dopant source, and their properties were investigated as a function of doping concentration. Increasing in boron concentration leads to reduction in peak intensity of (002) preferential orientation plane. Energy gap value of the films which is obtained from optical transmission measurements seems to shift to lower energy as the concentration dopant increases. However, the refractive index value increases as the boron concentration increases. When the boron content increases the sheet resistance value of $Cd_{0.6}Zn_{0.4}S$ thin films decreases rapidly in the dark and decreases slightly under illumination condition.

D_D0034 THERMAL DEGRADATION OF HIGH DENSITY POLYETHYLENE PLASTIC-FILM BY THERMOGRAVIMETRY

Chutima Paksunchai, Supreya Trivijitkasem, Chirawat Kluenrat and Rachanee Rujiwarodom.
* Department of Physics, Faculty of Science, Kasetsart University, Bangkok 10900, Thailand.
e-mail address: g4564081@ku.ac.th.

Abstract: Thermal degradation of high-density polyethylene (HDPE) plastic-film was studied by thermogravimetric analysis (TGA) at five different heating rates: 5, 10, 15, 20 and 30 K/min. The degradation of HDPE plastic-film occured in one step. The decomposition temperature of derivative thermogravimetric (DTG) curve was found to shift to higher temperature as the increased heating rate. The kinetic parameters were determined by Peak Property Method (PPM). The reaction order was not varied as heating rate, it was nearly equal to 1, while the activation energy and natural logarithm of pre-exponential factor of the plastic-film were decreased as the increased heating rate.

D_D0035 Preparation of Zinc titanate Nanostructures by Oxidation Reaction Technique

Surat Sedpho*, Pongsri Mangkorntong, Nikorn Mangkorntong and Supab Choopun
Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200 *E-mail address: sedpho@hotmail.com

Abstract: Zinc titanate nanostructures were prepared by oxidation reaction technique. Zinc and titanium oxide powder were mixed and screened on alumina substrate and sintered under oxygen atmosphere. The sintering temperature was varied from 600–900 °C for 6 hours. The obtained products were investigated by Field Emission Scanning Electron Microscopy (FE-SEM) for morphology and energy dispersive spectroscopy (EDS) for chemical composition. The diameter and length of zinc titanate nanostructures were in the range of 150-300 nm and 2.5-9 □m, respectively. The peaks in the EDS spectrum indicated that Ti was incorporated into ZnO and formed zinc titanate compound. These zinc titanate nanostructures could be explored for further applications such as gas sensor.

D_D0036 Preparation of ZnO Whisker by Growth from Vapor Method

Panupat Chaiworn*, Pongsri Mangkorntong, Nikorn Mangkorntong and Supab Choopun.
Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200
*Corresponding author E-mail address: master_Phy@hotmail.com

Abstract: ZnO whiskers were prepared by growth from vapor method. Zinc powder was heated at 600, 700 and 800 °C in the tube furnace for 2 hours under a normal atmosphere. The obtained whiskers were investigated by optical microscopy and Raman spectroscopy. The hexagon structure (pencil-like structure) was observed. The width and length of ZnO whiskers were in the range of 10-20 μm and 4-15 mm respectively. ZnO whiskers were investigated by optical microscopy, Field Emission Scanning Electron Microscopy for morphology and the Raman spectra confirmed that the obtained whiskers were zinc oxide, not zinc.

D_D0037 LENGTH MEASUREMENT BY ULTRASONIC SENSOR

Wittanee Hetrakul, Inthira Sripichai, Damras Pumnuan, Jukkrapun Nakjamsai, and Wandee Onreabroy
Department of Physics, King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand

Abstract: The ultrasonic distance measuring device combines latest ultrasonic sensor and microcontroller technologies. Microcontroller, PX-1000, is controlled by C programming language. With simple and single-handed operation, the device has been designed to increase flexibility and become more user-friendly. The mechanism of this measuring device is based on wave reflection and wave traveling time. The device measures the time it takes to transmit 40 kHz ultrasonic waves (Transducer) to the object and back to the receiver. The measured time is later used to calculate the distance between target and receiver. The measuring device yields output in both Metric and English unit. It can accurately measures distances from 0.10-4 meters. This device can store up to 4 outputs. Besides memory function, the backlight feature makes it easier to read in poor light condition.

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D_D0038 Direct enumeration of alloy configurations for semiconductor electronic structure properties

Sirichok Jungthawan, Sukit Limpijumnong
School of Physics, Suranaree University of Technology Nakhon Ratchasima, Thailand
Peter A. Graf, Kwiseon Kim, Wesley B. Jones National Renewable Energy Laboratory Golden, CO, U.S.A.
Gus L. W. Hart Department of Physics and Astronomy, Northern Arizona University Flagstaff, AZ, U.S.A.

Abstract: We present an approach to directly enumerating electronic structure properties of all possible zincblende-based alloy configurations whose unit cell contains up to a specified number of atoms. This method allows us to map the space of bandgaps and effective masses versus alloy composition and atomic configuration. We demonstrate for GaInP alloys that a large range of bandgaps and masses are available for a given composition. By decomposing the space of the possible atomic configurations into categories based on superlattice structure, we can identify trends in bandgap extrema. For example, bandgap maxima typically occur in [0 *h k*] superlattices where *h* is not equal to *k*, and minima typically occur in [1 1 1] superlattices. We focus on dilute GaInP and AlGaAs alloys where the minority composition is below 10 percent. The empirical pseudopotential method (EPM) is used to solve the single particle Schrödinger equation.

D_D0039 SOME PROPERTIES OF P -TYPE $CuAlO_2$ THICK FILMS PREPARED BY SCREEN PRINTING METHOD

Ngamnit Wongcharoen, Thitinal Gaewdang, Prathan Prachopchok*,Pakorn Sittiketkorn and Thitikorn Chanyatham
Department of Applied Physics, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Chalongkrung Rd., Ladkrabang, Bangkok 10520, Thailand;
*Corresponding author, E-mail ; p.t_physics@hotmail.com

Abstract: Polycrystalline of copper aluminium oxide ($CuAlO_2$) samples were prepared by a solid state reaction. The mixture of CuO and Al_2O_3 powders was fired at 1373 K for 24 h. Thick films of $CuAlO_2$ were deposited on glass substrate by screen printing method and using $CuAlO_2$ single phase in powder form as a precursor, dispersing them into acetone. The as-deposited thick films were annealed in air at 773 K for 24, 48, 72 and 96 h respectively. X-ray diffraction patterns of the as-deposited films show the peaks which could be assigned with those of the crystalline $CuAlO_2$ phase. The air -annealed films show the peaks of $CuAlO_2$ and CuO phases. As the increase in annealing time, the peak intensity of CuO phase also increases. Electrical resistivity measurements were performed on the air -annealed films with different annealing time. The activation energy of each films showing two values can be deduced from the variation of resistivity as a function of the inverse temperature. From the electrical properties of the air -annealed films, it may be indicated that the excess oxygen atoms within the annealed films play an important role on resistivity of the $CuAlO_2$ films.

D_D0040 Synthesis of $Mg_xZn_{1-x}O$ Nanostructures by oxidation reaction technique

Narongsak Yotmao, Pongsri Mangkorntong, Nikorn Mangkorntong, and Supab Choopun
Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200
E-mail address : Tong_phy@hotmail.com

Abstract: The nanostructures of $Mg_x Zn_{1-x}O$ were synthesized by oxidation reaction under a normal atmosphere. A mixture of Zinc powder and MgO (x = 0.05 – 0.30) powder were screened on alumina substrate. Then, the mixture was heated at temperature of 600–1000 °C for 6 hr. The nanostructures were characterized by Field Emission Scanning Electron Microscopy,

Energy Dispersive Spectroscopy for morphology and chemical composition, respectively. The nanostructures of $Mg_xZn_{1-x}O$ with size ranging from 250–950 nm, and length of several micrometers were obtained. The EDS spectrum suggested that Mg was incorporated into ZnO and formed $Mg_xZn_{1-x}O$ alloy.

D_D0041 GROWTH AND CHARACTERIZATION OF CdTe THIN FILMS PREPARED BY CLOSE -SPACED SUBLIMATION METHOD

Ng.Wongcharoen , T.Gaewdang , A.Hamwunggmoung*, P.Sriputtaiwon , P.Prachopchok
P.Sittiketkorn, T.Chanyatham and N. Promros
Department of Applied Physics, Faculty of Science, King Mongkut's Institute of Technology Ladkrabang, Chalongkrung Rd., Ladkrabang, Bangkok 10520, Thailand;
*Corresponding author, E-mail; adul_harn@yahoo.com

Abstract: CdTe thin films with different precursor-substrate spacer have been deposited by close-spaced sublimation (CSS) method on glass substrate in reaction chamber having low pressure about 2 0x 10^{-2} mbar. From XRD analysis, CdTe thin films are polycrystalline belonging to cubic structure with a preferential orientation of (111) plane. The strongest peak intensity of XRD is observed in the films prepared with precursor -substrate spacer being 6 mm. Energy gap value of the as-deposited films was evaluated from the optical transmission spectra. The lowest dark sheet resistance value of the films is obtained in the films prepared with the 6 mm precursor -substrate spacer. Regarding to our experimental results, it may be indicated that the 6 mm precursor -substrate spacer is the most suitable conditions in preparing CdTe thin films for solar cell application..

D_D0042 MEASUREMENT OF COHERENCE LENGTH OF LIGHT BY MICHELSON INTERFEROMETER

N. Ngernliang and P. Limsuwan
Department of Physics, King Mongkut's University of Technology Thonburi (KMUTT), 126 Prachautit Rd., Thungkru, Bangmod, Bangkok, 10140 Thailand
Email: opticslaser@yahoo.com, TEL:02-872-5253,02-470-8868 , FAX:02-872-5254

Abstract: In this research work, a Michelson interferometer has been applied for the measurement of coherence length of pure spectral line sources, i.e. mercury lamp and sodium lamp. The principle of coherence length measurement is based on the formation of interference fringes obtained from Michelson interferometer. In Michelson interferometer the light beam from a broad spectrum source is divided into two beams by a beam splitter. The two beams, are reflected at mirror M_1 and M_2 , and then interferes to form interference fringes as can be seen by the eye. The Michelson interferometer can be used to measure coherence length of light sources directly by measuring the largest difference in path length of the two mirrors over which we still observe fringe formation. By measuring the coherence length of the mercury green line and yellow line at wavelength of 546.1 nm and 579.0 nm, respectively; and the sodium D lines at average wavelength of 589.3 nm, the coherence lengths are 1.5, 1.7 and 0.6 mm, respectively. The measured values are in good agreement with those of calculated values (i.e. 1.49, 1.67 and 0.58 mm, respectively).

D_D0043 EFFECT OF ANNEALING TEMPERATURE ON THE PROPERTIES OF ITO FILMS PREPARED BY DC MAGNETRON SPUTTERING

K. Aiempanakit[1], S. Phutwat[1], S. Dumrongrattana[1], P.Rakkwamsuk[2]
[1] Department of Physics, Faculty of Science
[2] Division of Materials Technology, School of Energy and Materials King Mongkut's University of Technology Thonburi 126 Pracha Utit Road, Bangmod, Tungkru, Bangkok 10140, THAILAND
Email: Kamon_KMUTT@hotmail.com, Tel: 02-4708876, Fax: 02-4278785.

Abstract: Indium tin oxide (ITO) thin films were deposited on glass substrates without heating by dc magnetron sputtering using an In_2O_3-SnO_2 (90-10 wt%) target. The effects of annealing temperature on the structural and optical properties of the ITO films were studied. The ITO films for as-deposited were amorphous but after annealing the ITO films showed higher improvement of the crystallinity with increasing the annealing temperature. The average optical transmission in the visible region was higher than 80% for all films after annealed at 350°C while the average optical transmission in the near infrared region decreased with the increase in anneal temperature or increasing the film thickness. The energy gap of ITO increased with increasing the annealing temperature.

D_D0044 MONTE CARLO SIMULATIONS OF SIGNAL TRANSDUCTION MEDIATED BY G-PROTEIN: SPATIAL DISTRIBUTION OF MOLECULES.

Apiwat Wisitsorasak[1], Wannapong Triampo[1,2]
[1] Department of Physics, Faculty of Science, [2]Capability Building Unit in Nanoscience and Nanotechnology, Faculty of Science, Mahidol University, Bangkok 10400

Abstract: A critical question in signal transduction is what is the spatial distribution of involved species to optimize signal transduction processes. The purpose of this work is to investigate kinetics of all considered species including receptors and G-proteins in signal transduction mediated by G-proteins using direct Monte Carlo numerical simulations. The focus is on how each species redistribute or reorganize themselves to optimally achieve this transduction process. It was found that as increasing numbers of particles become large, they are transported into other particles domains and eventually, the system becomes globally completely disordered state. These results may suggest that in signal transduction process, the

molecules involved including receptors and G-proteins have tendency to reorganize themselves and become more uniformly disordered.

D_D0045 NUMERICAL ANALYSIS OF REFRACTIVE INDEX AND THICKNESS OF MULTILAYER FILM USING MICHELSON INTERFEROMETER

Pongsakorn Taloengtamrongkul[1], Nattapong Kaensa[1], Sunidsa Plangsungnurn[1], Siriwara Tosayanon[1], Onuma Noppagorn[1], Jarupat Disrattakit[1]

[1] Department of Physics, Faculty of Science, Srinakharinwirot University, Sukhumvit 23, Bangkok, Thailand.
E-mail: jarupat@swu.ac.th, Fax: (662)664-1000 Ext.8163

Abstract: A Michelson interferometer is basic optical instrument in the physics laboratory. Michelson's interferometer has become a widely used instrument for measuring extremely small distances. This equipment was applied to measure the thickness and the index of refraction of film. A glass plate, is coated by film, is inserted to the path of one of the beams of light traversing the arms of the Michelson interferometer. A glass plate in one of the arms is rotated, the path of the light will be increased, and the number of fringes corresponding to this change be observed. The results of numerical analysis represent the sensitivities of the Michelson interferometer. The sensitivities of detection of thickness changes and index of refractive are about 1 μm and 10^{-3}, respectively. The efficiency of measurement depends on the wavelength of the light source and resolution of the rotating state.

D_D0046 Preparation of Thin Film Crosslink Bovine Serum Albumin (BSA) on Gold Surface

Sukanya Petchsirivej[1,2,3], Boonsong Sutapun[4], Somboon Sahasitiwat[5], Toemsak Srikhirin[1,2]

[1] Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand
[2] Capability Building Center in Nanoscience and Nanotechnology, Faculty of Science, Mahidol University, Bangkok 10400, Thailand
[3] Department of Physical Science, Faculty of Science and Technology, Hauchiew Chalermprakiet University, Samutprakarn, 10540
[4] Electro-optic Laboratory, National Electronics and Computer Technology Center, Phratumtani, Thailand,12120
[5] Nationl Metal and Materials Technology Center, Pharatumtani, Thailand, 12120

Abstract: The main objective of this work is to prepare a crosslink BSA substrate for using as a covalent binding layer for Surface Plasmon Resonance (SPR) sensor. The preparation of crosslink BSA on the gold was done by varied volume of pre-crosslink BSA solution, from 10 to 600μL, which is spread on the 0.5 x 2.0 cm active area of the sensor. The measured optical thickness of the film was found to be increased as the volume of BSA is increased. The wettability of the crosslink is reduced as the surface coverage of the crosslink BSA on gold is increased. The surface coverage of the crosslink BSA on gold was found to be consistent with the observed data from contact angle and SPRs.

D_D0047 A STUDY OF SOL-GEL TRANSITION OF JELLY BY ULTRASONIC TECHNIQUES

Fuanglada Veerasai[1], Somsak Maneerattanakul[1], Srivikorn Dit-Udom-Po[2] and Surachate Krishsangchote[3]

[1] Department of Physics, Faculty of Science, Srinakharinwirot University, Wattana, Bangkok, Thailand
E-Mail: fuanglad@swu.ac.th, Somsak@swu.ac.th
[2] Department of Home Economics, Faculty of Science, Srinakharinwirot University, Wattana, Bangkok, Thailand
E-Mail: Srivikornd@yahoo.com
[3] Department of Physics, Mahidol Wittayanusorn School, 364 Moo 5, Salaya, Bhuddhamonthon, Nakhon Pathom, Thailand
E-mail: physicspurepure@hotmail.com, Fax: (662)849-7211

Abstract: This research was the study of the sol-gel transition of jelly by ultrasonic techniques. The purpose of this work was determined the mechanical properties of roselle jelly during the process of its sol-gel transition using 1 percentage weight of the sample element of jelly. The mixtures of the combination between κ-Carrageenan and Locust Bean Gum (LBG) from 6 samples, were between 0 - 1 percentage weight of LBG. The experiment was carried out in the temperature range 30°C - 70°C. The ultrasound was used in the frequency of 812 kHz in order to find the ultrasonic velocity (v) in the jelly. Its density (ρ) was obtained and the viscosity (η) was measured by the Brookfield Viscometer (RDVT II) for calculating shear modulus (G) which varied as the temperature and varied as the percentage of LBG. From the value of ultrasonic velocity (v), the density (ρ) and the shear modulus (G), the bulk modulus (B) of the jelly was calculated. The relations between bulk modulus of the jelly and the temperature, and the relations between bulk modulus of the jelly and percentage of LBG by weight were obtained in the form of numerical expression. The results indicated that the bulk modulus decreased linearly with increasing temperature, and slowly decreased non-linearly with increasing the percentage of LBG. The result of this study is consistent with Chen's research that when the percentage of LBG in jelly increased, the elastic modulus decreased non-linearly. By considering the changing rate of viscosity comparing with temperature, the gelation temperature was 46°C ± 2°C. This result was also consistent with Simeone's gelation temperature of 44 °C.

D_D0048 A STUDY OF SOL-GEL TRANSITION OF JELLY BY ULTRASONIC TECHNIQUES

Fuanglada Veerasai[1], Somsak Maneerattanakul[1], Srivikorn Dit-Udom-Po[2] and Surachate Krishsangchote3

[1] Department of Physics, Faculty of Science, Srinakharinwirot University, Wattana, Bangkok, Thailand
E-Mail: fuanglad@swu.ac.th, Somsak@swu.ac.th
[2] Department of Home Economics, Faculty of Science, Srinakharinwirot University, Wattana, Bangkok, Thailand

E-Mail: Srivikornd@yahoo.com
[3] Department of Physics, Mahidol Wittayanusorn School, 364 Moo 5, Salaya, Bhuddhamonthon, Nakhon Pathom, Thailand
E-mail: physicspurepure@hotmail.com, Fax: (662)849-7211

Abstract: This research was the study of the sol-gel transition of jelly by ultrasonic techniques. The purpose of this work was determined the mechanical properties of roselle jelly during the process of its sol-gel transition using 1 percentage weight of the sample element of jelly. The mixtures of the combination between κ-Carrageenan and Locust Bean Gum (LBG) from 6 samples, were between 0 - 1 percentage weight of LBG. The experiment was carried out in the temperature range 30°C - 70°C. The ultrasound was used in the frequency of 812 kHz in order to find the ultrasonic velocity (v) in the jelly. Its density (ρ) was obtained and the viscosity (η) was measured by the Brookfield Viscometer (RDVT II) for calculating shear modulus (G) which varied as the temperature and varied as the percentage of LBG. From the value of ultrasonic velocity (v), the density (ρ) and the shear modulus (G), the bulk modulus (B) of the jelly was calculated. The relations between bulk modulus of the jelly and the temperature, and the relations between bulk modulus of the jelly and percentage of LBG by weight were obtained in the form of numerical expression. The results indicated that the bulk modulus decreased linearly with increasing temperature, and slowly decreased non-linearly with increasing the percentage of LBG. The result of this study is consistent with Chen's research that when the percentage of LBG in jelly increased, the elastic modulus decreased non-linearly. By considering the changing rate of viscosity comparing with temperature, the gelation temperature was 46°C ± 2°C. This result was also consistent with Simeone's gelation temperature of 44 °C.

D_D0049 STUDY OF PHASE FORMATION AND DIELECTRIC PROPERTIES OF DYSPROSIUM OXIDE DOPED LEAD ZIRCONATE TITANATE CERAMICS.

Krit Koyvanich ,Supreva Triviittkasem, Ekachai Hoonnivathana, Phanom Kadrun
[1]Department of Physics, Faculty of Science, Kasetsart University, Bangkhen, Bangkok, 10900, Thailand.
E-mail:sornrams8@hotmail.com.

Abstract: 0.01mol % Dysprosium oxide doped lead zirconate titanate ceramics was investigated.The sintered density, at three sintered temperatures 1200,1250 and 1300°C, were nearly constant between 7.6-7.7 g/cm^3. The lattice parameters and cell volume of tetragonal phase from the first two sintered temperatures were nearly equal: a = 4.09 Å, c = 4.76 Å and V =79.9 Å^3. The c/a ratio was shrunk and cell volume was decreased at 1300°C sintering temperature. The PDZT ceramics sintered at 1300°C exhibited the best performance with high dielectric constant of 633.

D_D0051 GOLD - DOPED ZINC OXIDE NANOWIRES BY OXIDATION TECHNIQUE FOR ETHANOL SENSOR

Piboon Mongchey[1], Pongsri Mangkorntong[1], Nikorn Mangkorntong[1] and Supab Choopun[1]
[1] Department of physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200, Thailand.
E-mail:Pibomo@gmail.com

Abstract: Gold–doped zinc oxide nanowires and undoped ZnO nanowires were synthesized by oxidation technique and then, used to fabricate ethanol sensor to study ethanol sensing properties. The sensing properties were studied by measuring resistance change in air and in ethanol ambient with ethanol concentration of 50, 100, 200, 500, 1000 and 2000 ppm and at work temperature of 180-280 °C. It was found that at work temperature of 260 °C both sensors exhibit the highest sensitivity and the sensitivity of 5% gold-doped sensor shows slightly higher sensitivity at 2000 ppm.

D_D0052 THE SIZE EFFECT OF IRON CORE ON THEIR RELATIVE PERMEABILITY

Prasert Kengkan, Hong-vork Sinumnguypol
Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand
E-mail:25ex100445@kknet.co.th, Fax (6643)202374

Abstract: The affect of iron cores on magnetic field in a gap is studied. The dependence of relative permeability of these cores on their sizes are found. The basic concept used is that when equal currents are flown in the same direction in a pair of identical parallel coils placed with distance equal to their radii of curvature then magnetic field between these coils will be uniform, is used. The result of measurement is proved to be equal to the result of computer calculation using Biot-Savart law. When a pair of magnetic cores is placed in this uniform magnetic field, the induced magnetization current is considered as current in another pair of parallel coils. The same concept is used to measure and to calculate the relative permeability of iron cores. The results are 4.8, 4.4, 3.9 and 2.7 for the cores of diameter of 6.4, 7.0, 7.6 and 20.4 cm respectively.

D_D0053 Characterization of Electrical Discharges on Plasma Ozonizer System and Its Application

Pitchasak Chankuson[1] Supawan Tirawanichakul[2] and Yutthana Tirawanichakul[3]
[1,3] Department of Physics, Faculty of Science,
[2] Department of Chemical Engineering, Faculty of Engineering, Prince of Songkla University, Songkhla Thailand 90112
Corresponding e-mail address: Yutthana.t@psu.ac.th,

Abstract: Ozone gas is one of the strongest oxidizing agents. In recent years, ozone gas has been widely utilized in wastewater , drinking water and exhausted smoke, deodorization, color removal, and disinfection in industrial pipeline systems. Due to huge flux of dye wastewater from dyed Krajud mat village nearby Songkla lake, it affects some ecology system on site. Thus, objective of this work is to study the color removal of dyes wastewater from dyed mat village by ozone comparing

to that obtained by alum coagulation and the combination of ozonation and alum coagulation. The system is composed of dried air unit, high voltage power supply and ozoniser tubes. The configuration of the tube is type, "Cylindrical type" consist of two electrodes. The inner electrode is stainless steel, which is covered with Pyrex glass as the dielectric. The outer electrode is stainless steel. Oxygen gas is flowed through the discharge gap between the two electrode and AC high voltage power supply is supplied for ozone production. The amount of ozone produced is determined by the KI standard method. The result shows that the amount of ozone is proportional to the applied voltage. After varies the oxygen's flow rate from 6 to 10 L/min and considers the amount of ozone are approximately 41, 60, 80 and 135 mg/L at volumetric flow rate 8 L/min (discharged time 3 minutes) at 8, 9, 10 and 11 kV AC supply, respectively. The results show that amount of ozone produced was directly proportional to the input voltage and inlet air flow rate. Characteristics of effluents and ozone treated effluents were assessed in terms of the color removal efficiency is determined by light absorbance, biochemical oxygen demand (BOD) and chemical oxygen demand (COD). After treatment by these 3 methods, wastewater's the percentage of color removal can be reduced to approximately 56%, 62% and 35% , respectively. Its BOD can be reduced to approximately 64%, 70% and 54% ,respectively and COD can be reduced to approximately 78%, 81% and 62%,respectively. From the result, the most effective method for dye wastewater treatment is the combination of ozonation and alum coagulation. Moreover, the FTIR spectrograph illustrates that treated dye solutions has slightly difference compared to the reference sample. This is due to some of complicated functional groups (methylene, carboxylate etc.) are breakdown during ozonation.

D_D0055 STATIC AND DYNAMIC PROPERTIES IN RELAXOR FERROELECTRIC $KTa_{1-x}Nb_xO_3$ AND $K_{1-x}Li_xTaO_3$

D. La-Orauttapong[1] and J. Toulouse[2]

[1] Department of Physics, Faculty of Science, Srinakharinwirot University, Bangkok, Thailand.
E-mail:duangmanee@swu.com, Fax: (662)664-1000 ext.8551

[2] Department of Physics, Lehigh University, Bethlehem, PA, USA.

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Abstract: The relaxor behavior is characteristic of a number of mixed ferroelectric systems. Early explanation attributed it to a diffuse phase transition. Although all relaxors identified so far were lead-based systems, here, we propose lead-free $KTa_{1-x}Nb_xO_3$ (KTN) and $K_{1-x}Li_xTaO_3$ (KLT) as prototypes for the relaxors. In this study we have performed both neutron elastic and inelastic scattering to show the temperature dependence of both the diffuse and phonon scattering in KTN (x=17%) and KLT (x=16%). Both compounds show no broad diffuse scattering (no broad central peak at $\hbar\omega = 0$) in the transverse acoustic phonon region. Therefore, the effect of the diffuse component on phonons is expected to be minimal. Based on the measured temperature dependences of the transverse acoustic and transverse optic phonon energies, we infer that there is no strong coupling effect. These results are discussed in terms of the uncoupled harmonic oscillator.

D_D0056 METHODS OF DETECTING EXCESS Cu-Se COMPOUNDS IN $CuInSe_2$ EPITAXIAL FILMS.

Bancha Arthibenyakul, Panita Chinvetkitvanich, Chanwit Chityuttakan, Kajornyod Yoodee, Somphong Chatraphorn, Sojiphong Chatraphorn

Semiconductor Physics Research Laboratory, Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

Abstract: $CuInSe_2$ (CIS) heteroepitaxial thin films with varying Cu/In ratios have been grown on (001)-oriented GaAs substrates by molecular beam epitaxy (MBE). In the films with Cu/In ratios greater than unity, namely the Cu-rich films, the excess Cu-Se compounds grow epitaxially and simultaneously with the CIS films. The excess Cu-Se compounds are the unwanted materials in the fabrication of CIS-based thin film solar cells because they act like a metal. In this work, we use an atomic force microscopy (AFM), x-ray diffraction (XRD) and optical spectrophotometry as characterization methods for detecting the existence of Cu-Se compounds. We have found from the AFM-images that the surfaces of Cu-rich films show additional platelet-like features which are not observed in the near stoichiometric and the Cu-poor (Cu/In ratio<1) CIS films. The XRD spectra show broadening (004) and (008) peaks of Cu-rich CIS films. The AFM and XRD techniques cannot identify the existence of the Cu-Se compounds in the less-Cu-rich or near stoichiometric CIS films, whereas the optical reflection spectra in the near infrared range clearly show the metallic behavior of the excess Cu-Se compounds.

D_D0057 PENDULUM AND CHAOTIC MOTION

Prasert Kengkan2, Ratapol Promnoy

Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen, 40002, Thailand.
Email: 25ex100445@kknet.co.th, Fax: +66 43 202 374

Abstract: Rigid body pendulum motion under air resistant force with various initial conditions is studied both by computer programming and by experiment. The air resistant force is measured. The initial condition for the circular motion predicted from theory matches with the real experiment. The theoretical study is extended to cover forced oscillation to show resonance condition. The initial condition for chaotic motion is considered by using both phase diagram and Poincare section.

D_D0058 Fabrication of Matrix Organic Light Emitting Devices

Pairote Jaideaw[1,2*], Daranee Sridate[1], Thanida Chaiyapoom[1], Suthee Petcharavut[1], Malee Klinkulorb[1], Somporn Maneetoon[2] and Tanakorn Osotchan[2].

[1] Department of Physics, Faculty of Science and Technology, Phranakhon Rajabhat University, Bangkok 10220, Thailand.

[2] Capability Building Unit in Nanoscience and nanotechnology, Department Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.

Email: dangpai@hotmail.com

Abstract: In this research, matrix organic light emitting devices was fabricated with synthesized BEH-PF. The BEH-PF was coated on indium tin oxide (ITO) coated glass substrates. The ITO layer was etched in heated mixture of 30% nitric acid and 70% sulfuric acid at 60 °C for 15-20 second in order to obtain the sharp pattern of eight rows of 1×25 mm^2. The hole transport PEDOT:PSS layer was spin-coated on the ITO coated glass substrate at speed of 4000 rpm. The BEH-PF polymers layer was subsequently spun. The aluminum top electrode was coated by thermal evaporation in vacuum chamber under pressure below 10^{-4} Torr with the pattern of eight rows of 1×25 mm^2 which is cross to the ITO pattern. The current-voltage characteristic of the multi-layer device in vacuum exhibited an exponential curve with anti-symmetry between forward and reverse bias voltage. The turn on voltages for BEH-PF films was about 4.87- 5.25 V and the blue emitted light can be observed as that in peak wavelength of 467 nm in photoluminescence measurement. When increasing apply voltage to about 8-10 V, the neighbor pixel exhibits the blue light due to the high conduction at high electric field.

D_D0059 Adsorption of protein on functionalized polymer surfaces by surface plasmon resonance technique

Thidarat Wangkam, Sirasa Phoomkeaw, Toemsak Srikhirin[1] ,Boonsong Sutapun[2],Ratthasart Amarit[2], Somboon Sahasittiwat[3]
[1] Capability Building Unit in Nanoscience and Nanotechnology, Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.
[2] Electro-Optics section, National Electronics and Computer Technology Center (NECTEC) Pathumthani 12120,Thailand.
[3] National Metal and Materials Technology Center (MTEC) Pathumthani 12120,Thailand.
E-mail address: mvteddy@hotmail.com

Abstract: The adsorption of protein onto the polymer surface with different surface polarity was investigated by Surface Plasmon Resonance(SPR) technique. Polystyrene (PS) and copolymer at different densities of carboxyl group were coated on the gold film. The adsorption of Bovine serum albumin (BSA) protein was carried out by flowing the BSA solution onto the sensor surface at the constant flow rate. For the effect of BSA concentration at 0.001, 0.01,0.05, 0.1 ,0.5, 1 mg/ml , we found that SPR angle shift increase when concentrations increase and saturated at 0.1mg/ml.It showed that the adsorption process is controlled by concentration of protein. When we considered the effect of polarity, it show different orientation of polar on the surface.

D_D0060 A REAL-TIME VISUALIZATION OF BEHAVIOR OF COLLOIDAL PARTICLES IN AN AC ELECTRIC FIELD BY USING XGRAPHICS LIBRARY.

Chanpeng Angchakan 1 and Tanin Nutaro[1]
[1] Department of Physics, Faculty of Science, Ubon Rajathanee University, Warin Chamrab, Ubon Ratchanee, 34190
E-mail:tnutaro@yahoo.com, chanp2010@yahoo.co.th, Fax: 045 288 381

Abstract: We had performed a real-time visualization for studying the behavior of a solid-in-liquid colloidal system of mica spheres suspended in water under influence of an AC electric field. In our simulation the mica particles are uniform in size, with 1.5×10^{-6} m of radius, under uniformly 7500 V/m of electric field by using C programming and displays by Xgraphics library for X-Windows of Linux operating system. From the simulation we see, after 1.0×10^{5} time steps with $\Delta t = 0.001$ the particles were aligned forming stripes or chains, which is agree well with experiment.

D_D0061 THE VISUALIZATION OF SOLAR ENERGETIC PARTICLE TRANSPORT SIMULATION FROM THE SUN BY USING IBM DX

Tanin Nutaro[1]
[1] Department of Physics, Faculty of Science, Ubon Rajathanee University, Warin Chamrab, Ubon Ratchanee, 34190
E-mail: tnutaro@yahoo.com, Fax: 045 288 381

Abstract: We had performed computer simulations of Solar Energetic Particles (SEP) transport in radial outward from the Sun into heliosphere. After the simulation took place, we used the IBM Data Explorer (IBM DX), which is a high performance visualization package as a tool for studying the behavior of particle distribution in pitch angle cosine (m) and radial distance (r) in the evolution of time. We found that the simulation results agree very well with Ruffolo (1995) (1) and, we also found that the IBM DX is easy to use and suitable for a vast and complicate data interpretation.

D_D0062 Alcohol odor concentration effect on coated quartz crystal microbalance

Wiriya Suwannet[1], Rawat Jaisutti[1], Onanong Chamlek[1], Sirapat Pratontep[2], Teerakiat Kerdcharoen[1], Tanakorn Osotchan[1]
[1] Capability Building Unit for Nanoscience and Nanotechnology, Department of Physics, Faculty of Science, Mahidol University, Bangkok, 10400
[2] National Nanotechnology Center, Thailand Science Park, Patumtani,12120

Abstract: Coated quartz crystal microbalance was studied to examine the detection of various alcohol odors at the different concentrations. Eight types of alcohol including acetone, propanol, ethanol, tetrahydrofuran, methanol, nail remover, 100 pipers whisky and masterblend whisky were used in this experiment. Quartz crystals with resonance frequency of 2.000 MHz were coated with thin films of copper phthalocyanine by thermal vacuum evaporation technique. Two measuring chambers were used with volumes of 11.200 and 2.665 liters. The frequency measurement cycle is devided into three intervals. Initial frequency was measured for a half hour, after that the alcohol with various volumes of 0.1, 0.5, 1 or 5 ml was injected on the

filter paper in the chamber. The frequency was measured for three hours then the chamber was cleaned by turning the fan on to remove alcohol vapor for a half hour. In most cases, the frequency shift increases when the concentration of the alcohol vapor increase from 9 to 1,870 ppm. At high alcohol vapor concentration, the frequency shift exhibits four significant different features from eight types of alcohol. In some alcohol types, the increasing of frequency can be observed after alcohol injection at very high alcohol vapor concentration.

D_D0064 HOME BUILT PHOTON COUNTING SYSTEM FOR MOLECULAR LUMINESCENCE

Areefen Rassamesard, Jose H. Hodak, Tanakorn Osotchan,
Capability Building Unit of Nanoscience and Nanotechnology, Department of Physics, Faculty of Science, Mahidol University, Bangkok 10400, Thailand.
E-mail address: areefenmu@yahoo.com

Abstract: Photon counting circuits was constructed in-house in order to apply to measure the molecular luminescence. The designed system consists of fast amplifier for increasing the amplitude of photomultiplier tube (PMT) signal without delay time, discriminator circuit to select the desired voltage range to generate the pulse with constant nanosecond pulse width controlled by monostable circuit. The dark signal is an important factor for determine lower detection limit of photon counting system. The dark measurement results for Hamamatsu. PMT model 1P21 show that the dark count increases when the PMT supply voltage increases. However at supply voltage above 950 V the dark count dramatically increases and the 950 V was chosen for appropriate PMT supply voltage with dark count less than 100 Hz at lower level discriminator (LLD) of 30 mV. The maximum amplitude of dark count is 53 mV. This value is an important parameter used to set up reference LLD for our photon counting system. The photon count was also investigated and at the level of LLD of 30 mV the photon count rate of 10 kHz was achieved which has two orders of magnitude higher than the dark count. At the LLD value of with an appropriate setting, this system is able to detect fluorescence from molecules or fluorescent polymer chains.

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D_D0065 Kinetics of long-range ordering and magnetism of FePd alloy

Chaisak Issro[1], W. Püschl[2], W. Pfeiler[2], P.F. Rogl[3], and V. Pierron-Bohnes[4]
[1] Department of Physics, Faculty of Science, Burapha University, 20131 Chonburi, Thailand
[2] Institut für Materialphysik, University of Vienna, Strudlhofgasse 4, 1090 Vienna, Austria
[3] Institut für Physikalische Chemie, University of Vienna, Währingerstraße 42, 1090 Vienna, Austria
[4] IPCMS-GEMME, CNRS-ULP, 23 rue du Loess, BP 43, F-67034 Strasbourg Cedex 2, France

Abstract: The kinetics of long-range ordering and its influence a magnetism of FePd bulk thin foil and thin film were investigated. The thin foil was cold-rolled at room temperature to a thickness of about 10 μm and compared with results on a sort of 50 nm thick FePd thin films. FePd film on Si substrate was fabricated at room temperature by using dc and rf magnetron sputtering. Changes in long-range order (LRO) were studied by X-ray diffraction, electrical resisitivity measurement, and magnetic measurements. It is found that during isochronal heat treatment, the FePd phase of thin foil and sputtered film undergoes a phase transition from disordered face-centered cubic (fcc) to ordered face- centered tetragonal (fct) structure, showing a polycrystalline microstructure. From resistivity measurement it results that atomic jump processes in thin films occur similar to those in the thin foil sample. FePd films sputtered at room temperature initially are completely disordered but LRO starts during a subsequent temperature treatment below $T_{o/d}$.

D_D0066 THE COMPARATIVE STUDY OF THERMAL CONDUCTIVITY OF VARIOUS TYPES OF PRESSED-SOIL CEMENT BLOCK BY USING FINITE ELEMENT METHOD

Supon Sumran[1] and Chaweewan Chaiwattana[1]
[1] Department of Physics, Faculty of Science, Ubon Rajathanee University, Warin Chamrab, Ubon Ratchanee, 34190
E-mail:supon_sumran@yahoo.com, Fax: 045 288 381

Abstract: We have developed the lightweight pressed-soil cement block, which is a general purpose material for construction. The properties of this material we made are optimized between a highly compressive strength and a low thermal conductivity. Moreover, it has lightweight when compared to the ordinary pressed-soil cement that has ever been made. In this study, we made a prototype brick; as an indicator, by using the composition ratio of soil and cement of 7:1 (by volume). After that, we put the rice-husk ash with ratio 0.5, 1.0, 2.0, 3.0 to the main mixture for making various types of lightweight pressed-soil cement block and called, "B", "C", "D", "E" types, respectively ("A" is a prototype brick). Then we performed computer simulations by exploiting the thermal conductivity estimation method that was developed by Nutaro (1). We found that, the prototype brick (A) has thermal conductivity of 2.80 $W m^{-1}K^{-1}$ while all types of the lightweight brick give a lower thermal conductivity at about 1.98-2.25 $W m^{-1}K^{-1}$

D_D0067 AN EXPERIMENT TO STUDY STOKES' LAW AND TO DETERMINE THE VISCOSITY OF LIQUID BY USING ATWOOD'S MACHINE INTERFACED WITH MICROCOMPUTER

Piyarat Bharmanee, Pramot Satasuvon, Kheamrutai Thamaphat
Department of Physics, Faculty of Science,
King Mongkut's University of Technology Thonburi, Bangkok 10140, Thailand.
E-mail: s903607@yahoo.com, Tel: +66 24284209; fax: +66 28709837

Abstract: In this present work, Atwood's machine interfaced with microcomputer was used to investigate Stokes' law and

to obtain the magnitude of the viscosity of glycerin. Atwood's machine consists of two masses, m and M, connected by an inelastic massless string over an ideal massless pulley. When $m = M$, the machine is in stable equilibrium regardless of the position of the weights. On the contrary, when $m > M$, both masses experience uniform acceleration. Three steel spheres (m) of different masses and diameters were used. At each steel sphere, the data were obtained by varying the mass M and measuring the terminal speed. In each case, the experiment was repeated seven times at fixed glycerin temperature. Based on all of these data, the viscosity of glycerin can be calculated from the slope of graph of the terminal speed v versus the mass M. From the results, they found that the viscosity of glycerin at steel sphere m_1, m_2 and m_3 were 8.95, 9.74 and 9.00 poise, respectively. They indicated that the measured viscosity is related to the radius of the sphere.

D_D0068 INTEGRATION OF HUMIDITY AND TEMPERATURE SENSORS INTO AN ELECTRONICS NOSE SYSTEM

Rungroj Maolanon[1], Mario Lutz[2], Paisarn Daungjak na ayutthaya[3], Teerakiat Kerdcharoen[2], Sirapat Pratontep[1]
[1] Nation Nanotechnology Center, Nation Science and Technology Development Agency, Thailand Scienor Park, Pathumthani, 12120, Thailand
[2] Department of Physics, Faculty of Science, Mahidol University, Rama 6 Road, Bangkok 10400, Thailand
[3] Department of Physics, Institute of Science, Walailak University, Nakorn Si Thammarat, Thailand
Email: rungroj@nanotec.or.th

Abstract: An electronic nose is a biomimetic for distinguishing volatiles by analyzing patterns of responses from several gas sensors. One common problem of electronic noses is its sensitiveness in humidity and temperature. We have integrated a humidity and temperature sensor into an electronic nose system composed of metal oxide semiconductor gas sensors. The data acquisition was achieved by a home-built micro-processing unit that collects sensor voltage responses as digital data. These data will be then transmitted via a RS232 port for pattern analysis in a desktop computer system. For the test relative humidity from 40 - 80%, responses of some gas sensors increase with the humidity, whereas a reverse response was found in some other gas sensors. This finding should be beneficial in improving odor pattern recognition by the Principle Component Analysis (PCA) technique. In our future work, this electronic nose system will be applied in the quality control of fragrance and perfume.

D_D0069 RAMAN STUDY OF THE RELAXOR FERROELECTRIC (1-x)Pb($Zn_{1/3}Nb_{2/3}$)O_3-x$PbTiO_3$

Duangmanee La-Orauttapong[1], Tanaporn Tansakul[1], and Thanusit BurinPrakhon
[1] Department of Physics, Faculty of Science, Srinakharinwirot University, Bangkok, Thailand.
E-mail:duangmanee@swu.com, Fax: (662)664-1000 ext.8551
[2] Department of Physics, Faculty of Science, Khonkaen University, KhonKaen, Thailand.

Abstract: In this work we have performed the light Raman scattering on (1-x)Pb($Zn_{1/3}Nb_{2/3}$)O_3-x$PbTiO_3$ (PZN-xPT, x = 0 and 9%) in the wide temperature range between -75°C to 250°C and in the frequency range up to 1000 cm^{-1}. Basing on the Lorentzian peak fit of the scattering spectra, our results show that lowering the temperature leads to the appearance of the polar nanoregions (PNR's) characterized by off-center ions and to the slowing down processes of the re-orientational motion. The data presented here also suggest that the phonon Raman line at ~45 cm^{-1} did not agree with the phonon energies as measured by neutron scattering.

D_D0070 Optical Properties of CdS Nanoparticles Doped in Alumina Matrix by the Sol-Gel Method

Suriyong Pongpiboonkul, Kiranant Ratanathammapan, and Satrerat Hodak.
Department of physics, Faculty of Science, Chulalongkorn University, Phayatal Road, Bangkok, Thailand.

Abstract: Nano-sized CdS semiconductor particles in alumina matrix have been prepared by a sol-gel process which is used for applications in nonlinear optic. The sol was spun on cover-slide substrates with the speed of 4000 rpm for 120 sec, and then prepared at 120 °C for 120 sec. The deposition with spin coating procedures was repeated 5 layers. The samples were calcined at 300°C, 400°C, and 500°C for approximately one hour, after that gaseous H_2S was used to flow onto heated samples in order to convert CdO nanoparticles to CdS nanoparticles. Finally the samples were annealed at 300°C, 400°C, and 500°C for 20 min. The optical properties of the films were analyzed using optical absorption and photoluminescence spectroscopy. The correlation between the size of CdS nanoparticles and the film optical properties will be discussed.

D_D0071 DESIGN AND CONSTRUCTION OF MICROWAVE PLASMA REACTOR FOR DIAMOND FILM DEPOSITION

Nopporn Rujisamphan[1], Boonchoat Paosawatyanyong[1], and Vitaya Amornkitbamrung[2]
[1] Department of Physics, Faculty of Science, Chulalongkorn University, Phayatai Road, Bangkok, Thailand.
[2] Department of Physics, Faculty of Science, Khon Kaen University, Mittraphab Road, Khon Kean, Thailand.

Abstract: We have designed and constructed a mode-adjustable microwave plasma reactor. The system can be divided into two main parts; (a) a vacuum chamber constructed from number 304 stainless steel cylinder with an outside diameter of 219 mm and a height of 254 mm, (b) a power coupling module consisting of a 2.45 GHz 1.4 kW magnetron power supply and applicator (waveguide, waveguide plunger, and a cylindrical cavity). An air-filled aluminium rectangular waveguide WR340 (86.4×43.2 mm^2) was designed and constructed to guide the microwave with TE_{10} mode. The brass antenna is used to convert the TE_{10} mode in WR340 waveguide to the TM_{01} mode in cylindrical resonator at 2.45 GHz resonant frequency. The antenna is located at a quarter guide wavelength from the short end of the adjustable waveguide plunger where the

standing wave produces a maximum electric field. The plasma is formed inside of a bell-jar quartz placed inside the cylindrical resonator. The reactor will be used for diamond film deposition. The preliminary results of films and plasma parameters such as electron temperature and plasma density will be presented.

D_D0072 FABRIC AND FIBER MODIFICATION USING RADIO FREQUENCY PLASMA PROCESS.

Thidarat Supasai[1], Satreerat K. Hodak[1] and Boonchoat Paosawatyanyong[1]
[1] Department of Physics, Faculty of Science, Chulalongkorn University, Phayatai Road, Bangkok, Thailand.
E-mail: pumthidarat@hotmail.com.

Abstract: We have studied the hydrophobicity improvement of fabrics using radio-frequency (RF) inductively coupled SF_6 plasma. The plasma was generated in the pressure of 0.005-1 torr and with the RF power of 25-75 watts. A set of fabrics including polyethylene terephthalate (PET), mixed Thai silk, Thai silk and cotton are treated under different operating conditions. Treated fabrics were characterized by scanning electron microscopy, water contact angle and absorption time measurement as a function of storage time after treatment. The atomic species in SF_6 plasma were measured by optical emission spectroscopy (OES). The results show spectrum line of F I in SF_6 plasma which is believed to increase the hydrophobicity of fabrics. Compared with untreated fabrics, treated fabrics improve the absorption time from 0-30 mins to about 200 mins depending on the types of fabrics, and the contact angles significantly increase about two times. The suitable operating conditions were at pressure of 0.5 torr and RF power of 50 watts.

D_D0073 CRYSTAL STRUCTURE AND MORPHOLOGY OF $BaTiO_3$ / $SrTiO_3$ POLLYCRYSTALINE FILMS PREPARED BY A SOL-GEL METHOD

Supha Sirinam[1] Satreerat K.Hodak *,Kiranant Ratanathammapan[1], Jose Hector Hodak[2]
[1,*]Department of Physics, Faculty of Science, Chulalongkorn University, Phayatai Road, Bangkok ,Thailand.
[2] Department of Physics, Faculty of Science, Mahidol University, RamaVI Road, Bangkok,Thailand.
* Satreerat.H@chula.ac.th

Abstract: We have fabricated polycrystalline $BaTiO_3$ (BTO) and $SrTiO_3$ (STO) on silicon substrates by a sol-gel method. The prepared suitably solutions were deposited on Si substrates by the spin-coating technique at 4000 rpm for 4 minutes. After preheating at 120 °C for 20 minutes, the films were heated at different temperatures (300 °C, 800 °C, 1000 °C). The crystal structure and morphology of the both film types were analyzed by using atomic force microscopy and X-ray diffractometry techniques, respectively. We found that both BTO and STO films heated at 300 °C did not show the crystalline structure. The both types of films heated at 800 °C showed the grain size of 50 nm. BTO film prepared at 1000°C showed the grain size of 80 nm which is smaller than that of STO film with the grain size of 100 nm prepared at the same temperature. From X-ray diffraction measurement, BTO prepared at 800 °C and 1000 °C presented the (100) (110) (111) (200) (201) and (211) planes. An extra peak indicating TiO_2 peak was found in BTO prepared at 1000 °C. The STO film prepared at 800 °C and 1000 °C showed the peak of the (100) (110) (111) (200) (210) and (211) planes. The optimum heating temperatures for BTO and STO films are at 800 °C and 1000°C, respectively.

E_E0001 SINTERING AND CHARACTERIZATION OF THE $Pb(Zr_{0.52}Ti_{0.48})O_3$ CERAMICS WITH Bi_2O_3 ADDITIVE

Soosuek Roobliem, Anuson Niyompan* and Rungnapa Tipakontitikul
Department of Physics, Faculty of Science, Ubon Ratchathani University, Warinchamrap, Ubon Ratchathani, 34190 Thailand.
E-mail:anuson@rocketmail.com, Fax: (664) 528-8381

Abstract: Lead zirconate titanate (PZT) powder was prepared by conventional method and then sintered using Bi_2O_3 1 wt.% as a sintering additive. It has been observed that presence of Bi_2O_3 can lower the sintering temperature and also enhanced the densification of PZT ceramics. High dense PZT ceramic with Bi_2O_3 1 wt.% was obtained by sintering at 1035 °C for 4 h. with trace amount of the secondary phase.

E_E0002 MICROSTRUCTURE DEVELOPMENT OF THE Cu_2O-DOPED PZT CERAMICS DURING SINTERING PROCESS

Rungnapa Tipakontitikul*, Soosuek Roobliem and Anuson Niyompan
Department of Physics, Faculty of Science, Ubon Ratchathani University, Warinchamrap, Ubon Ratchathani, 34190 Thailand.
E-mail:rungnapa@rocketmail.com, Fax: (664) 528-8381

Abstract: Microstructure development during sintering process of the compacted Lead Zirconate Titanate ceramics with and without presence of Cu_2O were investigated. During sintering, constant heating/cooling rates and dwell time were applied. The influence of sintering temperature on the final microstructure, phase formation and linear shrinkage were studied. Normal grain growths with lower shrinkage were observed for the PZT ceramics that without doping. Meanwhile, introduction of Cu_2O (1 wt.%) induced an abnormal grain growth but the growth rate determined by linear shrinkage were accerelated. Presence of Cu_2O was lower the sintering temperature and enhance degree of microstructure development.

E_E0003 SYNTHESIS OF NANOCRYSTALLINE MIXED OXIDES OF Ni/Mg/Zr

Wimonrat Trakarnpruk[1]*, Charnsak Sukkaew[2]
[1] Green Chemistry Research Unit, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand. e-mail:wimonrat.t@chula.ac.th, Fax: (662)2187598
[2] Petrochemistry and Polymer Science, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

Abstract: Ni/Mg/Zr mixed oxides were prepared from $Ni(NO_3)_2$, $Mg(NO_3)_2$ and $ZrO(NO_3)_2$ aqueous solution using four methods: coprecipitation (CP), citrate precursor technique (CT), modified citrate precursor (MCT) and citrate precursor/ethylene glycol (MCTE). The molar ratios of citric acid to metal ion and citric acid to ethylene glycol were varied. The structures of the oxides prepared under various conditions were examined by X-ray diffraction (XRD), Fourier-transform infrared (FTIR), transmission electron microscopy (TEM), and Brunauer-Emmet-Teller (BET) methods. The XRD results showed that when molar ratio of Mg/Zr 1/4 and 15% wt Ni, the mixed metal oxide exists as cubic Mg-ZrO_2 phase. In the CP method in which calcination was performed at 600°C, oxides possessed surface area of 136 m^2/g and small pore size. In the CT method in which calcination was performed at 800°C, the oxides had very low surface area and pore size. Two calcinations were performed in the MCT method, it yielded oxides with high surface area (145 m^2/g) and large pore size. The MCTE method also yielded oxides with high surface area (144 m^2/g). The powder oxides from all methods have particle sizes in the range of nanometer.

E_E0004 (NATURAL DYEING BY INORGANIC THIN LAYER TECHNOLOGY)

Pajaera Patanathabutr[1]*, Nisarat Taweewan[1], Ploy Leaungphairojana[1], Volker Rossbach[2]
[1]*Department of Materials Science and Engineering, Faculty of Engineering and Industrial Technology, Silpakorn University, Nakorn Pathom, 73000, Thailand
[2] Department of Polymer and Textile Chemistry, University of Technology TU Dresden, D-01062, Germany

Abstract: Inorganic Thin Layer Technology (ITLT) was applied to natural fiber to reduce amount of metal mordants in natural dyeing. ITLT allows the application of bilayer structure mordants. The first layer of silicon dioxide, formed by Sol-Gel process of Tetraethoxysilane (TEOS) in aqueous media, was mechanically anchoring on fiber surface. The chemically bound second layers of a transition metal chelate bound with natural dyes. This research aims to study dyeing efficiency of ITLT treated natural fibers. Natural dyes of stems of *Caesalpinia sappan* Linn., leaves of *Terminalia catappa* Linn., and fruits of *Diospyros mollis* Griff. with metal mordants of Alum ($Al(NH_4)(SO_4)_2.12H_2O$) and Copper Sulfate ($CuSO_4.5H_2O$) were used to dye mulberry silk and cotton woven fabrics. It was found that ITLT technique can improve dye absorption of natural fibers and improve light fastness and washing fastness of natural dyed fabrics for approximately 1 level up. Inductively Coupled Plasma (ICP) analysis showed that ITLT technique can reduce amount of metal mordants in dye bath, on average, from 1% to 0.03% by weight of fabrics. Moreover, ITLT can improve metal mordants absorption, on average, by 80% of original metal mordants in dye bath, so less amount of excess metal mordant would be left in waste water from dyeing process. It was found that the average metal content in dyed ITLT fabrics was only 0.02% by weight of fabrics. Color spectrophotometer showed that the use of different metal mordants led to different shades of dyed fabrics.

E_E0005 ADHESION STRENGTH OF Al-12Si AND Ni-5Al THERMALLY SPRAYED COATINGS ON DIFFERENT SURFACES

Sukanda Jianslrisomboon[1], Anucha Watcharapasprn[1] and Sittichai Wirojanupatump[2]
[1] Department of Physics, Faculty of Science, Chiang Mai University, 50200, Thailand

[2] Department of Chemistry, Faculty of Science, Chiang Mai University, 50200, Thailand
Corresponding author, e-mail: sukanda@chiangmai.ac.th

Abstract: This research studied a suitable coating for improving surfaces of 'One Tambon One Product (OTOP)' products. The main purpose of this research is to study the adhesion strength of thermally sprayed Aluminium-12 wt% Silicon (Al-12Si) and Nickel-5 wt% Aluminium (Ni-5Al) coatings which were adhered onto cast sand and ceramic by using flame spray technique. The results showed that the adhesion strength between coating and substrate depended on substrate surface roughness. The Al-12Si coating had higher adhesion strength compared to Ni-5Al coating. Apart from this, the polished surface of Al-12Si coating was shinier than the Ni-5Al coating. This indicated the beauty of the Al-12Si coating over the Ni-5Al coating; thus the Al-12Si is suitable for decoration of the OTOP products.

E_E0006 PHASE FORMATION AND MICROSTRUCTURE OF PZT/WO_3 NANOCOMPOSITE CERAMICS

Sukanda Jiansirisomboon, Tharathip Sreesattabud and Anucha Watcharapasorn
Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai, 50200, Thailand.
Corresponding author, e-mail: sukanda@chiangmai.ac.th

Abstract: This research studied the effects of an addition of nano-sized WO_3 particles on phase formation and microstructure of PZT ceramic. PZT/xWO_3 powders where x = 0, 0.5, 1, 3 and 5 vol% were prepared by a conventional mixed-oxide method through ball milling, freeze-drying, pressing and sintering at 1200°C for 2 hr at a heating/cooling rate of 5°/min. The experimental results showed that the change of tetragonal phase to rhombohedral phase was more pronounced with increasing the WO_3 content. The densities of the PZT ceramics were found to increase with addition of WO_3 and the high relative densities could be maintained up to the maximum amount of WO_3 used. Apart from this, the WO_3 particles had a direct effect on grain size reduction in the nanocomposite ceramics.

E_E0007 IN-FLIGHT, SPLAT AND COATING MICROSTRUCTURE RELATIONS OF COMBINE WIRE ARC SPRAYED Zn/Al12Si COMPOSITE COATINGS

Budsarakam Phangsee[1], Sittichai Wirojanupatump[2] and Sukanda Jiansirisomboon[1]
[1] Department of Physics, Faculty of Science, Chiang Mai University, 50200, Thailand
[2] Department of Chemistry, Faculty of Science, Chiang Mai University, 50200, Thailand
Corresponding author, e-mail: lamyai_phy@yahoo.com

Abstract: In-flight, splat and coating microstructue relation of combine wire arc sprayed Zn/Al12Si composite coatings compared with Zn and Al12Si wires were investigated in this work. The result showed that the mean diameter of splat diameter depended mainly on in-flight particles. Two types of splat morphologies were found, this was related to coating microstructure. A near disk-like shape splat morphology with no splashing found in the microstructure of Zn coating, which fine splats and dense lamella structure were found. Arc sprayed Al12Si wire formed flower-like splats presented dense splat morphology as a result of fully molten in-flight particles. Furthermore, Zn/Al12Si coating showed coarser lamella structure resulting two types of splats.

E_E0008 FABRICATION AND PHASE FORMATION OF PLASMA SPRAYED Al_2O_3-TiO_2 NANOCOMPOSITE COATINGS

N. Dejang[1], S. Wirojanupatump[2], A. Watcharapasorn[1] and S. Jiansirisomboon[1]
[1] Department of Physics, Faculty of Science, Chiang Mai University, Chiang Mai 50200
[2] Department of Chemistry, Faculty of Science, Chiang Mai University, Chiang Mai 50200
Corresponding author: n_dej@hotmail.com

Abstract: This research aimed to fabricate thermal sprayed Al_2O_3-xTiO_2 (x = 0, 3, 13 and 20 wt%) nanocoposite coatings. Starting with the preparation of nanocomposite feedstock powders by a simple wet milling process using the Al_2O_3 (22-45 μm) and nano-sized TiO_2 (50 nm) powders for 5 h, dried and sieved the mixed powders before spraying onto a mild steel substrate using a plasma spray technique. Phases and their changes were investigated using X-ray diffraction technique. The results showed that the phases of both Al_2O_3 and TiO_2 compounds were changed. The reaction between these two phases also occurred due to excessive heat from plasma spraying.

E_E0010 KINETIC OF CATIONIC CYCLIZATION IN DEPROTEINIZED NATURAL RUBBER LATEX BY USING A NOVEL CATALYST

Sa-ad Riyajan, Jitladda Sakdapipanich
[1] Department of Polymer Science, Faculty of Science, Prince of Songkla Univeristy, Hat Yai, 94100, Thailand
[2] Department of Chemistry, Faculty of Science, Mahidol University, Bangkok, 10400, Thailand
[3] Insititute of Science and Technology for Research and Development, Mahidol University, Salaya Campus, Nakornpathom, 73170, Thailand

Abstract: The property of natural rubber (NR) is more interesting, excepting for some properties need to improve. The cyclization reaction is an interesting reaction for modified NR to thermoplastic elastomer. Cyclization of deproteinized natural rubber (DPNR) or purified NR latex was effectively performed in latex phase by using trimethylsilyl-trifluoromethane sulphonate or trimethylsilyltriflate (TMSOTF). Various cyclization conditions affecting on degree of cyclization were studied such as