EDITORIAL

During 2009, and especially on November 11-15, the Facultad de Ciencias Químicas, Universidad de Concepción, celebrated its 50 Anniversary. The origin of our Faculty is the foundation of the Instituto Central de Química at 1959, during the period of the Rector David Stichkin. The first Director was Prof. Juan Perelló Puig. Subsequently, Professors Orlando Pavez, Pablo Dobud, Juan Bartulin, Germán Acuña, Moisés Silva, Sergio Quadri, and Bernabé L. Rivas have been Directors or Deans. During 1980 the Instituto Central de Química was changed, giving place to the Facultad de Ciencias and then during 1993 the current Facultad de Ciencias Químicas was created, formed by 5 Departments, Department of Analytical and Inorganic Chemistry, Department of Organic Chemistry, Department of Physicochemistry, Department of Polymers, and Department of Earth Sciences. There are three careers, Licenciado en Química-Químico, Químico Analista, and Geología and also three graduate programs, Doctor in Ciencias c/m Química which is the oldest program of the Universidad de Concepción, Magister en Ciencias c/m Química, and Doctor in Ciencias Geológicas. The academic and non-academic staff are formed by 122 persons. All the academics have a full time contract, and 85% possess a master or doctor degree. For the first time our Faculty has developed the teaching and research activities at an excellent level contributing to the regional and national development. Normally, the academics are teaching more than 30 careers for 8000 undergraduate students/year. The Graduate programs have about 30 students/year, a 20-25% come from other countries. The Doctor Program en Ciencias c/m Química has formed above 90 young scientists. The research is developed with the important financial support coming from different international and national agencies or programs, contributing to the high level human resources formation, patents, and papers. Our faculty has also contributed significantly to the development of the chemistry and has been strongly related with the Sociedad Chilena de Química, SChQ, contributing from different points of views and serving several charges. Thus, an important number of members of SChQ are academics of our faculty, as well as the Presidents: Professors Otto Weinnert, José Baabor, Mario Suwalsky, Bernabé L. Rivas, J. Guillermo Contreras, Galo Cárdenas, and Patricio Reyes. On behalf of all the personnel of our Faculty, I thank very much to the Sociedad Chilena de Química to dedicate a special issue to our 50 Anniversary.

Dr. Bernabé L. Rivas Q.
Dean
Facultad de Ciencias Químicas
Universidad de Concepción
STRUCTURAL EFFECTS OF VERAPAMIL ON CELL MEMBRANES AND MOLECULAR MODELS

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Scanning electron microscopy of intact human erythrocytes incubated with verapamil indicated that they underwent morphological alterations. Fluorescence spectroscopy on isolated unsealed human erythrocyte membranes showed an increase of the anisotropy and generalized polarization. X-ray diffraction on dimyristoylphosphatidylcholine and dimyristoylphosphatidylethanolamine bilayers showed a perturbation of the polar head and acyl chain regions of both lipid bilayers. Human neuroblastoma cells incubated with verapamil suffered a sharp decrease of cell viability.

SYNTHESIS AND CHARACTERIZATION OF Zn(II) COMPLEX WITH THE ACETATE AND OROTIC ACID MIX LIGANDS

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Semi-empirical calculations on the orotic acid structure have been carried out. The optimised structure was compared with those crystallographic data in order to analyze the reliability of the data and its use in the semi-empirical calculations of the structure of the obtained compound from orotic acid with Zn(II) acetate.

CRYSTAL STRUCTURE STUDY OF 1-(2-FURYL)-3-(3-METHYL-2-THIENYL)-PROPENONE, C₁₂H₁₀O₂S

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The 1-(2-furyl)-3-(3-methyl-2-thienyl)-propenone, C₁₂H₁₀O₂S, was synthesized and determined its structure. Their most interesting aspects are to be found in their interatomic interactions, of varied type (C—H···O, C—H···π, π···π) and strength.

key words: propenone, crystal structure, π—π contacts, H-bonding

CLASSIFICATION OF GENOTYPES OF EUCALYPTUS GLOBULUS UNDER COLD CONDITIONS USING THEIR FREE AMINO ACIDS CONTENT ON LEAVES AND REGULARIZED DISCRIMINANT ANALYSIS (RDA)

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Regularized discriminant analysis (RDA) were used to classify genotypes of Eucalyptus globulus by cold resistance using samples’ foliar damages and amino acid content of leaves.
HYDROGELS FROM ACRYLIC ACID WITH N,N'-DIMETHYLACRYLAMIDE: SYNTHESIS, CHARACTERIZATION, AND WATER ABSORPTION PROPERTIES

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Copolymer hydrogels of acrylic acid (AA) with N,N'-dimethylacrylamide (NNDMAAm) were synthesized by solution free radical polymerization at different feed mole ratios. They were characterized by elemental analysis, FT-IR spectroscopy, thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and contact angle.

The phase transition temperature of these copolymers’ aqueous solutions increased when the hydrophilic AA moiety content increased in the copolymers. The monomer reactivity ratios for poly(AA-co-NNDMAAm) are \( r_1 = 0.650 \) and \( r_2 = 1.160 \), \((r_1 \times r_2 = 0.753)\). The effect exerted by reaction parameters, including the concentration of cross-linking reagent, the monomer concentration, pH, temperature, salt solutions, and solvent polarity on the water absorption, were also studied. Under the experimental conditions, the copolymer poly(AA-co-NNDMAAm) 0.5 mol-% MBA with a feed mol ratio 3:1 presents the highest swelling properties, 544 g water/ g xerogel.

ENANTIOSELECTIVE HYDROGENATION OF 1-PHENYL-1,2-PROANODIONE ON Pt/ZrO\(_2\) CATALYSTS

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The enantioselective hydrogenation of 1-phenyl-1,2-propanedione at 298K and pressure of 40 bar of H\(_2\) over different zirconia supported Pt catalysts has been studied. The catalysts were characterized by nitrogen adsorption-desorption isotherms at 77 K, hydrogen chemisorption, XRD and TEM techniques. The reactions were carried out in a stainless steel batch reactor using cyclohexane as solvent and cinchonidine as chiral modifier. The presence of CD in the reaction medium is necessary to induce an enantioselective excess (ee) of the desired product, that is R-1-phenyl-1 hydroxi-2-propanone. In all the studied systems, the relation between the enantioselectivity and the CD concentration added in situ exhibits a bell type curve, indicative of the importance of competitive adsorption between the modifier and the substrate on the catalyst surface. On the other hand, confinement effect led to an important enhancement in the activity in those catalysts supported on mesostructured supports, mainly in the Pt/CNTsZrO\(_2\) catalyst.

POLY(SODIUM-10-UNDECYLENATE) AS PSEUDO-STATIONARY PHASE IN THE SEPARATION AND QUANTIFICATION OF POLYAROMATIC HYDROCARBONS BY MICELLAR ELECTROKINETIC CHROMATOGRAPHY

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Different molar mass fraction of poly(sodium-10-undecylenate) (PSU), were tested as pseudostationary phase in the separation of a mix of 4 polyaromatic hydrocarbons (PAHs) by Micellar Electrokinetic Chromatography (MEKC). Limit of Detection (LOD) and Limit of Quantification (LOQ) for 4 PAHs were calculated from the calibration curves in optimal separation conditions.
HYDROCARBONS SYNTHESIS FROM A SIMULATED BIOSYNGAS FEED OVER Fe/SiO\textsubscript{2} CATALYSTS

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Fischer Tropsch reaction using a mixture similar to that obtained from biomass transformation has been studied on Fe/SiO\textsubscript{2} catalysts. The CO conversion over Fe/SiO\textsubscript{2} catalysts and distribution of liquid hydrocarbons are mainly determined by the dispersion of Fe species and average size of iron particles respectively.

SPIN-ORBIT AND SOLVENT EFFECTS IN THE LUMINESCENT [Re\textsubscript{6}Q\textsubscript{8}(NCS)\textsubscript{6}]\textsuperscript{4-}, Q = S, Se, Te CLUSTERS: MOLECULAR SENSORS AND MOLECULAR DEVICES

RODRIGO RAMÍREZ-TAGLE\textsuperscript{1}, LEONOR ALVARADO-SOTO\textsuperscript{1}, LUCIA HERNÁNDEZ-ACEVEDO\textsuperscript{1} AND RAMIRO ARRATIA-PÉREZ\textsuperscript{*}

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Relativistic time-dependent density functional (TDDFT) calculations including spin orbit interactions via the zero order regular approximation (ZORA) and solvent effects using the COSMO model were carried out on the [Re\textsubscript{6}Q\textsubscript{8}(NCS)\textsubscript{6}]\textsuperscript{4-},(Q = S, Se, Te) clusters. These calculations indicate that the lowest energy allowed electronic transitions are characterized by being of LMCT type. The calculated absorption maximum tends to shift to longer wavelengths as the face-capping chalcogenide ligand becomes heavier. Thus our calculations predict that the [Re\textsubscript{6}Se\textsubscript{8}(NCS)\textsubscript{6}]\textsuperscript{4-} cluster might be also luminescent. Due to the unusual properties exhibited by these and other isoelectronic and isostructural hexa Re and hexa Mo clusters we proposed here the design of molecular sensors for detecting volatile organic contaminants and molecular nanocells for molecular electronics.

EFFECT OF Ag ADDITION ON THE THERMAL STABILITY AND CATALYTIC PROPERTIES OF LAFEO\textsubscript{3} PEROVSKITE

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Two important effects upon Ag substitution in a pure LaFeO\textsubscript{3} perovskites were observed: i) a greater reduction ability, ii) higher occurrence of oxygen vacancies due to β-oxygen desorption, which were not active in the studied reaction.

THEORETICAL STUDY OF THE NON-WATSON-CRICK BASE PAIR GUANINE-GUANINE

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A theoretical study of the non canonical base pair, Guanine-Guanine (G-G) has been carried out in the frame of molecular orbital theory using density functional theory (DFT). The Becke three parameter hybrid including correlation functional that contains local and non-local terms (B3LYP) was used thoroughly. The 6-31G(d,p) basis set was employed to obtain the optimized geometry and energy of the non-Watson-Crick pair formed between two molecules of guanine. The results compare well with the properties of other base pairs of biological interest. At the DFT level the non-planarity of the pair is evident. The two guaines molecules are bent by ca 12\degree and buckled. The interaction energy corrected by BSSE is equal to -10.7 kcal / mol, similar to that calculated for other pairs involving bases of nucleic acids.
ONLINE MULTI-STAGE MEMBRANE FILTRATION OF SYNTHETIC POLYDISPERSED WATER-SOLUBLE POLYMERS WITH UV VISIBLE ABSORPTION AS A MODE FOR THEIR DETECTION

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This paper reports the application of online membrane filtration with UV visible absorption as a mode of polydispersed substances detection. It was also used the combination of MF and GPC to provide more complete information about the molecular weight distribution of the obtained fractions.

THE INHIBITION ACTION OF ETHYL-2-PHENYL HYDROZONO-3-OXOBUTYRATE ON THE CORROSION OF 6061 AI ALLOY/ SiCp COMPOSITE IN HYDROCHLORIC ACID MEDIUM

U ACHUTHA KINI*, PRAKASH SHETTY*, S DIVAKAR SHETTY, ARUN ISLOOR, RAMADEV HERLE*


Polarization techniques and weight loss method are used to study the inhibition effect of oxobutyrate on the corrosion of Al alloy/SiCp composite in HCl medium. Oxobutyrate acts as an effective cathodic inhibitor. Inhibition takes place through adsorption mechanism and it follows Temkins and Langmuir isotherms.

ELECTRON TRANSFER RATES OF ALKYL–FERROCENE MOLECULES FORMING INCOMPLETE MONOLAYER ON SILICON ELECTRODES

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This study shows the results obtained when binding alkyl ferrocene molecules on silicon surface forming incomplete monolayers, employing a new and versatile synthesis route. Three redox active molecules have been employed in this study: Propyl–ferrocene, pentyl–ferrocene and decyl–ferrocene. XPS and electrochemical characterization have been realized. Electron-Transfer rates were determined by AC voltammetry technique, showing that kinetic constant is independent of the length of the alkyl chain employed in the modification.

ELECTROCHEMICAL OXIDATION OF IODIDE AT A GLASSY CARBON ELECTRODE IN METHYLENE CHLORIDE AT VARIOUS TEMPERATURES

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Electrochemistry of iodide was investigated in 0.1M TBAP/ CH₂Cl₂ using cyclic voltammetry, convolution transforms voltammetry, chronoamperometry and chronopotentiometry techniques at a glassy carbon electrode (GCE) at various temperature ranging from -20 °C to 21 °C. It was found that electrooxidation of iodide proceeds as ECEC scheme. The accurate test of the parameters evaluated experimentally was verified by comparing the experimental voltammograms with the simulated one.
NEW AMIDES OF SULPHONAMIDES: SYNTHESIS AND BIOLOGICAL EVALUATION

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A series of new amides of sulphonamides were synthesized through one-pot reaction and evaluated for their antiinflammatory, ulcerogenic and antibacterial activities with some significant results.

QUANTUM CHEMICAL STUDY ON THE MECHANISM OF THE ADDITION REACTION BETWEEN GERMYLENE AND EPOXYETHANE

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The mechanism of addition reaction between germylene and epoxyethane has been investigated employing B3LYP/6-311+G* method. Two reaction pathways have been predicted. Additionally, the orbital interactions are also discussed for the leading complex.

Ni(II) REMOVAL BY BIOSORPTION USING FICUS RELIGIOSA (PEEPAL) LEAVES

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The sorption equilibrium was established in about 60 minutes with equilibrium capacity of 6.35 ± 0.54 mg/g. The Ni(II) sorption is highly dependent on pH and maximum removal was observed at pH 7 above which metal started to precipitate. Evaluation of experimental data in terms of biosorption kinetics showed that the biosorption of nickel (II) on biomass followed pseudo-second order kinetics.

DETERMINATION OF ANTIPARKINSONISM DRUG ENTACAPONE

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Two spectrophotometric procedures are presented for the determination of the antiparkinsonism drug entacapone. The first method based on the formation of a coloured complex of entacapone with ferric chloride, which could be quantified spectrophotometrically at 665nm. The second Spectrophotometric method determine entacapone in presence of levodopa and carbidopa (which formulated with entacapone in stalevo tablets) by measuring the UV absorbance of entacapone either in zero order at 391nm or in the first order by measuring the amplitude between 360nm and 402nm without any interference from levodopa and carbidopa. HPLC method is described for the separation and determination of entacapone, levodopa and carbidopa on Luna CN 150 x 4.6 column with UV detection at 390nm for entacapone and at 280nm for both levodopa and carbidopa.

INVESTIGATING THE COMPATIBILITY OF POLYMERS IN COMMON SOLVENT

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The viscosity of polyblend is a good indication of compatibility of polymers. The viscosity at different shear rates and concentration of polymer solutions is plotted against polyblend composition of Poly(methyl methacrylate)/Polyethylene glycol. At 40 % blend composition the viscosity shows a minimum, indicating a phase inversion between the two polymers, as shown in the figure.
A VALIDATED DENSITOMETRIC METHOD FOR ANALYSIS OF TELMISARTAN AND ATORVASTATIN CALCIUM IN FIXED DOSE COMBINATION

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High-performance thin-layer chromatographic method for analysis of Telmisartan and Atorvastatin calcium (silica gel 60 F\textsubscript{254} as stationary phase and toluene: methanol 7: 3, v/v as mobile phase) in fixed dose combination has been developed.

AN INEXPENSIVE AND CONVENIENT PROCEDURE FOR CHLOROMETHYLATION OF AROMATIC HYDROCARBONS BY PHASE TRANSFER CATALYSIS IN AQUEOUS MEDIA

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An inexpensive, efficient, and convenient procedure in which aromatic hydrocarbons are directly converted to the corresponding chloromethylated products catalyzed by ZnCl\textsubscript{2}/AcOH/H\textsubscript{2}SO\textsubscript{4}/PEG-800 in aqueous media under PTC conditions has been developed.

CHALCONSEMICARBAZONE: A NEW SCAFFOLD FOR ANTIPELLEPTIC DRUG DISCOVERY

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In present time a new class aryl semicarbazone is emerged as new pharmacophore in epileptic drug discovery having broad spectrum activity. We have applied hybridization of pharmacophore strategy of drug design and developed a new pharmacophore. We have synthesized and done their pharmacological screening for the protection of seizures, behavioral study and CNS activity. The compound 1-[1-(2,4-dihydroxyphenyl)-3-(2-hydroxyphenyl)allylidene]-4-(2-fluorophenyl) semicarbazide (8) emerged as the most active prototype molecule in all the models.

SECONDARY METABOLITES ISOLATED FROM THE FUNGUS MONASCUS KAOLIANG-FERMENTED RICE

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A chemical study of the EtOAc-soluble ethanolic extract of Monascus kaoliang BCRC 31506 (Eurotiaceae) fermented rice led to the isolation of a new furan-3-one derivative along with 9 known compounds, monascin (2), ankaflavin (3), N-trans-feruloyltyramine (4), vanillic acid (5), 4-acetonyl-3,5-dimethoxy-p-quinol (6), (+)-β-eudesmol (7), trans-phytol (8), aesculetin dimethyl ether (9) and (-)-matairesinol (10). Structure 1 is proposed for monascuskaoliangine on the basis of spectroscopic evidence (NMR, UV, IR, and HRMS). None of the compounds exhibited significant scavenging activity toward DPPH radical in bioautography or spectroscopic assays.
STYRENE/STYRENE-DERIVATIVE COPOLYMERIZATION BY Ph$_2$Zn-METALLOCENE-MAO SYSTEMS: HOMO- AND COPOLYMERIZATION OF STYRENE WITH α-METHYLSTYRENE.

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Styrene/α-methylstylene copolymers were synthetized, through coordination polymerization, using binary metallocene-MAO and ternary Ph$_2$Zn-metallocene-MAO initiator systems. For the metallocenes used the efficiency follows the order IndTiCl$_3$ > Cp$_2$TiCl$_2$ > (n-BuCp)$_2$TiCl$_2$, with the half-sandwich metallocene IndTiCl$_3$ showing greater efficiency than the true metallocenes. Both electric and steric effect on comonomers much influenced copolymerization process.

SIMULTANEOUS DETERMINATION OF EMTRICITABINE AND TENOFOVIR BY AREA UNDER CURVE AND DUAL WAVELENGTH SPECTROPHOTOMETRIC METHOD

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Fig. (1). Overlay spectra of Tenofovir in methanol: (1) 6 µg/mL; (2) 12 µg/mL; (3) 24 µg/mL; (4) 36 µg/mL; (5) 48 µg/mL and Emtricitabin (A) 4 µg/mL; (B) 8 µg/mL; (C) 16 µg/mL; (D) 24 µg/mL; (E) 32 µg/mL.

Simple, precise and accurate Area under curve (AUC) and Dual wavelength methods were developed for the simultaneous estimation of tenofovir and emtricitabine in combined dosage form. Emtricitabine shows maximum absorbance at 281 nm and Tenofovir shows maximum absorbance at 259 nm. For the AUC method, the wavelength ranges between 242-248 nm and 269-275 nm were selected with reference to the absorbance curves plotted between the wavelengths of 200-400 nm. In the second method i.e. Dual wavelength method in which two wavelengths were selected for each drug in a way so that the difference in absorbance is zero for another drug. The accuracy of the proposed method was checked by recovery studies, by addition of standard drug solution to preanalysed sample solution at three different concentration levels (50 %, 100 % and 150 %) within the range of linearity for both the drugs. The repeated sample study was done to observe the intra-day and inter-day precision. From the analysis of the marketed tablet preparation, the percent label claim of analytes was estimated.

13- EPI-NEOCLERODANES FROM BACCHARIS MARGINALIS

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In addition to the known diterpenes, desoxystauriculin and dihydrotrucumanoic acid, a new neoclerodane diterpene was isolated from Baccharis marginalis.

CARBON DIOXIDE ACTIV ATION BY Y ATOM AND Y$^+$ CATION IN THE GAS PHASE: A DENSITY FUNCTIONAL THEORETICAL STUDY

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In the reaction between Y$^+$ cation and CO$_2$, the minimum energy reaction path is found to be neither on the triplet PES nor on the singlet one. Instead, the minimum energy reaction path requires the crossing of two adiabatic surfaces with different spin states. Specifically, the reaction starts on the triplet PES and ends on the singlet PES.
ANODIC SYNTHESIS, SPECTRAL CHARACTERIZATION AND ANTIMICROBIAL ACTIVITY OF NOVEL 2-AMINO-5-SUBSTITUTED-1,3,4-OXADIAZOLES IN THE NON AQUEOUS MEDIUM

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Synthesis of 2-amino-5-substituted-1,3,4-oxadiazoles through the electrochemical oxidation of semicarbazone was carried out at platinum anode at room temperature under controlled potential electrolysis in an undivided cell assembly.

PREPARATION AND CHARACTERIZATION OF CHITOSAN/AGAR BLENDS: RHEOLOGICAL AND THERMAL STUDIES

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Abstract

In this work, a number of mixture aqueous solutions of chitosan/agar (CS/AG) at different ratios (considering chitosan as the main component) were prepared. The rheological properties i.e. shearing viscosity and shear stress of the blend solutions as a function of shear rate was investigated. Among the parameters studied were temperature, shearing time and storage time. Results showed that almost Newtonian behavior was observed at temperatures from 40°C to 55°C for the ratios 100/0, 90/10, 80/20 and 70/30. However, the proportions 60/40 and 50/50 showed a clear shear thinning behavior (pseudoplastic non-Newtonian behavior). It was also found that all the blend solutions obeyed the Arrhenius equation. In addition, the effect of shearing time on the dynamic viscosity of all blends did not show any significant differences at all shearing times applied in this study except the proportion 50/50 wherein decreasing in shearing viscosity and shear stress was observed as the shearing time increased. Furthermore, different behaviors were observed for the blend solutions when the period of storage was extended to three weeks. The thermal properties of the blend films was also studied in this work. The differential scanning calorimetry (DSC) curves showed that the interaction between chitosan and agar may occur.

DIFUNCTIONAL SILARYLENE-CONTAINING ALIPHATIC COMPOUNDS. SYNTHESIS AND CHARACTERIZATION OF BIS(p-(CARBOXYMETHYL)PHENYL)(R)PHENYLSILANE AND BIS(p-(2-AMINOETHYL)PHENYL)(R)PHENYLSILANE (R= Me, Ph)

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Diphenylacetic acids and phenethylamines containing a silarylene moiety were obtained from a common precursor: dibenzyl nitrile. This last was obtained after the synthesis of the respective ditolyl and dibenzyl bromide derivatives. All compounds were characterized by IR-TF, ¹H, ¹³C and ²⁹Si NMR.

PHENOLIC CONTENTS AND ANTIOXIDANT ACTIVITY IN CENTRAL-SOUTHERN URUGUAYAN PROPOLIS EXTRACTS

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Nineteen samples of Uruguayan propolis were analyzed by RP-HPLC and its antioxidant capacity by Antiradical Activity Determination (DPPH) and Microsomal Lipid Peroxidation (MLP) assays, showing all of them have good antioxidant properties. As shown in the image, it is noteworthy the greater abundance of flavanones and flavones (like pinocembrin and chrysin, respectively) in all samples.
FORMATION OF HIERARCHICAL CuO NANOWIRES ON A COPPER SURFACE VIA A ROOM-TEMPERATURE SOLUTION-IMMERSION PROCESS

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In this paper, we report on the synthesis of CuO nanowires arrays on copper plate using a simple wet chemical method at room temperature and the effect of heat treatment on the final surface morphology. TEM images show CuO nanowires grown onto copper substrate. The bright field image show in the figure a reveals that the growth of the nanowires in the sample under heat treatment is caused by the coalescence process of the started CuO. High resolution TEM image shows in figure b confirmed that the nanowires presented exhibited the CuO phase.

ADSORPTION MECHANISM OF BENZOTRIAZOLE FOR CORROSION INHIBITION OF COPPER-NICKEL ALLOY IN HYDROCHLORIC ACID

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The inhibition of copper corrosion by Benzotriazole (BTA) in 5% HCl has been investigated by weight loss technique at different temperatures. Langmuir adsorption isotherm, Freundlich Adsorption Isotherm and Kinetic-Thermodynamic Model were used to describe the adsorption process depending on values of surface converge. Maximum value of surface converge was 0.998 for BTA at 35 °C and 15 g/l inhibitor concentration, while the lower value was 0.868 at 55 °C and 1 g/l inhibitor concentration. The films formed on the copper-nickel alloy surface of BTA appeared to obey the Langmuir Adsorption Isotherm more than Freundlich adsorption isotherm. In the other hand, results showed that the Kinetic-Thermodynamic Model was unsuitable to fit the experimental data of the BTA of the present study.