



JDD2023 :8-9 Mai 2023

nouveaux complexes cationiques du Nickel à ligands iminopyridine, synthèse et caractérisation

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Commission : chimie

Salle : 2

Mots clés : ligands iminopyridine, complexes cationiques de Nickel, synthèse, caractérisation

Abstract :

une série de ligands iminopyridine (L1, L2, L3) ont été synthétisés et caractérisés par des analyses spectroscopie IR, UV, RMN 1H et RMN 13C. Ces ligands réagissent avec(DME) NiBr₂ dans le dichlorométhane ou THF, pour donner des complexes de Nickel(II) et l'addition oxydant de sel de methallyl (C₁H₇OP(N(Me)₂)₃) (PF₆) sur un composé zéro valent du Nickel formé in situ abouti à la formation du complexes de Nickel (I).



JDD2023 :8-9 Mai 2023

Macrocycles tetraaza combinés : Synthèse, Caractérisation, Complexation par des Ions Fe(II) et Co(II)

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Commission : chimie

Salle : 2

Mots clés : Macrocycles tetraaza combinés : Synthèse, Caractérisation, Complexation par des Ions Fe(II) et Co(II)

Abstract :

Dans cette étude, nous avons réussi à synthétiser un tétraazamacrocycle base de Schiff (N₄) de formule chimique C₄₀H₂₄N₄ et le complexer par la suite par des métaux de transitions MCl₂.xH₂O où M=Fe (II) et Cobalt (II), suivie d'une substitution des contre ions Cl⁻ par l'Acide ParaToluèneSulfonique (APTS) induisant ainsi des complexes octaédriques stables. Les complexes obtenus sont caractérisés par H¹NMR, ¹³C, UV-Vis, FT-IR et analyse thermique par calorimétrie différentielle à balayage DSC.



JDD2023 :8-9 Mai 2023

Synthesis, characterization and photophysical properties of new functional phénanthrene derivatives

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Commission : chimie

Salle : 2

Mots clés : Phenanthrene, Photooxidation, Absorption, Fluorescence

Abstract :

Helicenes and their homologues represent a class of polyaromatic hydrocarbons consisting of orthoannellated benzene nuclei with a non-planar topology. Due to their unique helical structure, helicenes often exhibit interesting electronic [1] and chiroptical properties [2]. They find applications in catalysis [3] and in asymmetric synthesis [4] as well as in light-emitting diodes [5]. Here we report the synthesis of several new functional phenanthrenes that could be used as precursors for different helicenes. The compounds are grafted with donor and acceptor functional groups at selected positions on the aromatic rings, with the aim of using them to access helicenes and to examine their optoelectronic properties. The compounds were obtained in good yields through a short photochemical approach involving mild and easy experimental conditions. The absorption properties of these compounds have been explored experimentally in various solvents showing a strong absorption wholly in the UV spectrum ($\lambda_{\max} = 281\text{--}285\text{ nm}$). These compounds exhibited blue or red-shifted emissions resulting in quantum yields of 0.07 to 0.21. Their electrochemical properties have been also investigated to assess the HOMO and LUMO energy levels which allow an electrochemical band gap ($E_{\text{g-el}}$) ranging between 2.19 eV to 2.74 eV.



JDD2023 :8-9 Mai 2023

Photooxidation pathway providing 15-bromo-7-cyano[6]helicene. Chiroptical and photophysical properties

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Commission : chimie

Salle : 2

Mots clés : Chirality, Helicenes, Photolysis, Enantiomeric resolution, Photophysical properties

Abstract :

15-bromo-7-cyano[6]helicene, has been prepared, in good yield, through a two step-sequence starting from 2-bromobenzo[c]phenanthrene-6-carbonitrile and making use of palladium-catalyzed Heck coupling and oxidative photocyclization. Optical resolution of the racemic helicene has been achieved, providing both enantiomers in high optical purity (>96.5% ee). The organic material exhibited a blue emission, and HOMO and LUMO energy levels were estimated experimentally, demonstrating an electrochemical band gap of 2.36 eV. Quantum chemical investigations based essentially on DFT and TD-DFT are discussed to more exploit the geometrical and electronic properties of the new helicene.



JDD2023 :8-9 Mai 2023

Synthesis, characterization and structure study of a new hybride organic-inorganic polyoxovanadate compound

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Commission : chimie

Salle : 2

Mots clés : Polyoxovanadate, X, Ray diffraction, FTIR, Hirschfield surface and UV, Vis

Abstract :

Hybrid solids that combine both metal-oxide and organic ligand “building blocks” are a growing class of new materials that are beginning to receive widespread attention because of their potential to express, within the same compound, both the physical properties of metal oxides in conjunction with the versatility and chemical flexibility of organic ligands. This chemical synergy can yield new routes to a plethora of novel structures and properties with many potential applications, such as in those explored for absorbent, catalytic, and sensor-related properties. New polyoxovanadates with organic cations, $(C_2H_{10}N_2)[VO_3]_2$, was synthesized. This compound are isolated and characterized in the solid state and in solution by elemental analysis, powder X-Ray diffraction, FTIR, DSC, electrochemical proprieties and UV-Vis. Further confirmation of the structures was obtained by single-crystal X-ray diffraction studies. The Hirshfeld surface analysis was performed to confirm that within the intermolecular interactions occurring in the crystal, the $O \cdots H/H \cdots O$, $O \cdots O$ and $H \cdots H$ interactions dominate. This compound crystallized in a monoclinic system, P21/c space group with the cell parameters: $a = 5.05455(3) \text{ \AA}$, $b = 12.7741(6) \text{ \AA}$, $c = 5.7116(3) \text{ \AA}$, $\beta = 97.774^\circ$.



JDD2023 :8-9 Mai 2023

Experimental and Theoretical Study of the Structure and Dynamic of Tetradecyltrimethylammonium Bromide (TTAB) micelles in water

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Commission : chimie

Salle : 2

Mots clés : Micelle TTAB/ Constante de Micellisation/ Conductivité/ Théorie d'Onsager, Kim

Abstract :

In this work, the conductivity of Tetradecyltrimethylammonium bromide “TTAB” ($C_{17}H_{38}NBr$) in aqueous solution was measured in water at $25^{\circ}C$ and 1atm, in a large range of concentration: $1.2 \cdot 10^{-3} \text{ mol.l}^{-1} \leq C(TTA^{+}) \leq 2.5 \cdot 10^{-2} \text{ mol.l}^{-1}$. TTAB micelles are formed above their corresponding critical micellar concentration ($CMCTTAB = 3.62 \cdot 10^{-3}M$), resulting from the spherical association of a fraction of the monomers (TTA^{+}) proportional to their corresponding degree of micellization $(1-\beta)$. In addition, micelles are partially neutralized by the condensation of Br^{-} counterions, so that the apparent charge number of each micelle is equal to: $Z_{app} = ZS(\alpha - \beta)/(1 - \beta)$, where ZS is the structural charge number (equal to the aggregation number), and $(1 - \alpha)$ is the degree of the ionic condensation. Experimental results were analyzed according to our coherent model, the generalization of the Fuoss ionic-association model and the Onsager–Kim–MSA conductivity theory of mixed electrolytes, in order to determine the thermodynamic constant of micellization and the conductivity at infinite dilution of TTAB micelles, and taking into account the dielectric friction effect on micelles. It results from coupling processes; between frictions due to ionic relaxation; that monomers are accelerated while counterions and micelles are slowed down during their migration.



JDD2023 :8-9 Mai 2023

electrochemical sensor for iron (III) detection based on (E)-2-((phenylimino)methyl) phenol modified platinum electrode

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Commission : chimie

Salle : 2

Mots clés : (E), 2, ((phenylimino)methyl) phenol, iron (III), optical propriety, impedimetric sensor, DFT calculation.

Abstract :

The critical role of ferric ions in biological systems, as well as the health impact posed to humans by related toxicity caused by the consumption of iron-contaminated drinking water or food, as well as exposure to other environmental sectors, necessitate the development of a sensitive method for determining these ions in a variety of domains such as medical uses, biological and environmental samples. The measurement of ferric ions was explored using a new impedimetric sensor based on the bases Schiff molecule, (E)-2-((phenylimino)methyl) phenol (E-PNMP). UV-vis assessed the capacity of E-PNMP to identify ferric ions, indicating that we obtained a complex E-PNMP /Fe³⁺ with a stochiometry. (1:2). Electrochemical impedance spectroscopy was used to characterize the E-PNMP modified electrode. (EIS). Under ideal conditions, the suggested impedimetric sensor has a detection limit of 2.49.10⁻¹² M in the concentration range of 10⁻¹² M to 10⁻⁵ M. As a result, the examined impedimetric sensor demonstrated excellent sensitivity, selectivity, reproducibility, and repeatability. A Pt/E-PNMP electrode was successfully used to measure iron (III) in an actual sample. A computational analysis with DFT employing the B3LYP functional and the 6311++G (d, p) basis set was also carried out to further understand the sensing mechanism of E-PNMP/iron.



JDD2023 :8-9 Mai 2023

An electrochemical enzyme-free glucose sensing based on a novel Cs/Cu-MOF composite

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Commission : chimie

Salle : 2

Mots clés : Metal, organic frameworks, Chitosan, Amperometric glucose sensors

Abstract :

Metal-organic frameworks (MOFs) represent promising materials, endowed with interesting properties such as large surface area, chemical versatility, availability of active functional groups, showing broad application prospects such as in bio-sensing, catalysis and gas adsorption [1]. In this work, a new electrochemical non-enzymatic glucose sensors was designed and constructed by using Cs/Cu-MOF modified Screen-printed carbon electrode. The electrocatalytic properties of the Cs/Cu-MOF fabricated electrode towards the electro-oxidation of glucose was evaluated by using cyclic voltammetry and amperometry analyses. Different effective parameters on the performance of the electrochemical sensor, including KOH concentration, applied potential, repeatability and selectivity, were investigated. Under optimized conditions, the novel sensor shows excellent electro-activity with a linear range of 0.4 μ M-1500 μ M and a low detection limit of 0.4 μ M with a high sensitivity of 945.94 μ AmM⁻¹cm⁻² and a good selectivity. Furthermore, this sensor was successfully applied for the detection of glucose in real sample.



JDD2023 :8-9 Mai 2023

Chemical composition and evaluation of insecticidal activity of *Thapsia garganica* L. seed essential oil against *Tribolium castaneum*

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Commission : chimie

Salle : 2

Mots clés : *Thapsia garganica*, Essential oil, chemical composition, pest management.

Abstract :

Recently, the use of essential oils as natural insecticides has shown significant potential for the pest management . The present study was conducted to investigate for the first time the chemical composition and insecticidal activity of the essential oil isolated by hydrodistillation from the seeds of *Thapsia garganica* L. (Apiaceae family). Gas chromatography coupled to mass spectrometry (GC/MS) and to flame ionization detector (GC-FID) were used for the qualitative analysis and quantification of the volatile constituents. 1,4-Dimethylazulene (51.3%) was identified as the main compound of the essential oil. Concerning the repellent effect, results revealed that seed essential oil was strongly repellent towards *Tribolium castaneum* adults (PR = 100% after 2 h) and highly toxic reaching 93.3% mortality after 24 h of exposure. These encouraging outcomes suggested that the essential oil of *T. garganica* could be considered a potent natural alternative to residual persistent and toxic insecticides.



JDD2023 :8-9 Mai 2023

Regioselective, One-Pot Synthesis, DFT and Molecular Docking Studies of Novel Conjugates barbituric acid as anti-inflammatory Agents

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Code : 469125

Commission : chimie

Salle : 2

Mots clés : Keys words: barbituric acid, isoxazole, anti, inflammatory activity, DFT calculation, molecular docking.

Abstract :

The discovery of new biologically active molecules represents a main objective in the field of medicinal chemistry. 1,3-dipolar cycloaddition is one of the most commonly used reactions in organic chemistry. For that, we made our contribution to the preparation of new poly-heterocyclic molecules built around barbituric acid and various aryl nitro oxides using click chemistry as methodology. We synthesized a new series of barbituric acid linked isoxazoles via a regioselective 1,3-dipolar cycloaddition reaction. This cycloaddition was carried out between the di(1-propargyl) barbiturate 1 and the aryl nitro oxide precursors 2(a-g), in different solvents in the presence of Et₃N and catalyzed by CuI to give new cycloadducts 3(a-g) with good yields (Scheme 1). In addition, a DFT-based study was also performed to explain the reactivity behaviors of some of the products. To understand the activity and the mechanism of action, we examined the binding modes of the two representative ligands, using the molecular docking program AutoDock vina. All the above findings consolidated by the proven results of in vitro anti-inflammatory activity, indicate that the derivatives barbituric acid bearing isoxazole moiety derivatives may be a potent inflammatory inhibitor.



JDD2023 :8-9 Mai 2023

Chemical composition, insecticidal and Allelopathic activities of the fractionated essential oil extracted from the resin exuded by *Araucaria heterophylla*

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Commission : chimie

Salle : 2

Mots clés : *Araucaria heterophylla*, Essential oil, Fractionation, Chemical composition, Insecticidal, Allelopathic.

Abstract :

The essential oil (EO) of the resin of the Tunisian *Araucaria heterophylla* ecospecies was investigated for its chemical composition and tested for insecticidal and allelopathic activities. The essential oil was extracted using hydrodistillation for 9 h (yield of 4.2% w/w). A fractional hydrodistillation with time intervals of three hours leading to 3 fractions was carried out in order to facilitate the chemical identification and to locate the studied biological activities. GC-FID and GC/MS analysis of the EO and its fractions allowed the identification of the majority of the constituents which consisted predominantly of hydrocarbon

sesquiterpenes, oxygenated sesquiterpenes and hydrocarbon diterpenes. Twenty-five volatile compounds were identified in the *A. heterophylla* essential oil, including α -Copaene (10.8%), α -Copaen-11-ol (7.8%), spathulenol (10.5%), 15-Copaenol (8.2%), Ylangenal (10.3%), Dehydrosaussurea lactone (7.7%) and sandaracopimaradiene (11.4%) as the major compounds. The second part aimed to study the insecticidal and allelopathic activities which led to good results.



JDD2023 :8-9 Mai 2023

Bioactive compounds from *Cynara scolymus* bracts: Physico-chemical characterization and biological evaluation

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Code : 469275

Commission : chimie

Salle : 2

Mots clés : *Cynara scolymus*, polysaccharide, polyphenols, biological evaluation.

Abstract :

Currently, the recovery of bioactive compounds from natural sources has received considerable attention because of their potential use as ingredients in food, pharmaceutical, and cosmetic formulations [1]. Among these compounds, polyphenols and polysaccharides have been the most studied in recent studies [2]. The first part of this study concerns the extraction and the physico-chemical characterization of polysaccharides from two varieties of *Cynara scolymus* (L.) bracts: Blanc Oranais (PSG) and Violet d'Hyères (PSV). The polysaccharides were characterized by IR-TF, SEC and RMN 1H. The results showed that PSG and PSV are RG-I pectins. The two polysaccharides were then biologically evaluated. In the second part we investigated the phenolic composition of the ethanolic extracts from the two studied artichoke varieties using LC-MS. The colorimetric assays showed that the two fractions are rich in total polyphenols and flavonoids. Importantly, the two ethanolic extracts have interesting antioxidant and antidiabetic activities.



JDD2023 :8-9 Mai 2023

Towards antibacterial derivatives of maslinic and oleanolic acids

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Code : 469514

Commission : chimie

Salle : 2

Mots clés : Olea europaea L., Maslinic acid (MA), Oleanolic acid (OA), quinolones, 1, 3, Dipolar Cycloaddition, Triazoles

Abstract :

Maslinic acid (MA) and oleanolic acid (OA) are key compounds from *Olea europaea* L. and as most of hydroxy pentacyclic triterpene acids (HPTAs), they exhibit a wide spectrum of biological activity. [1] Herein, we report an effective procedure for the chemical modification of isolated MA and OA through the synthesis of new 1,4-disubstituted-1,2,3-triazoles (3a, b). This procedure involved azides (1a, b) originated from natural MA and OA and a series of propargylated quinolones and fluoroquinolones (2) throughout the Cu-catalyzed azide-alkyne cycloaddition (CuAAC) forming the triazolo bridge between the natural and the synthetic part of synthesized hybrid compounds.



JDD2023 :8-9 Mai 2023

Synthesis and characterization of new functional benzo[c]phenanthrene derivatives

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Salle : 2

Mots clés : Helicenes, Photolysis, Cyclization, Photooxidation, Optical properties, Organic Semiconductors

Abstract :

A variety of functional benzo[c]phenanthrene derivatives were synthesized in good overall yield under mild experimental conditions. These derivatives were obtained by oxidative photocyclization of suitably substituted 1,2-diarylethylenes bearing reactive functional groups and were characterized by ¹H, ¹³C and COSY NMR, mass and IR. The absorption and fluorescence properties of the target compounds were examined in solution and a strong absorption in the UV region as well as a strong blue emission were observed.



JDD2023 :8-9 Mai 2023

Development of an electrochemical sensor based on f-MWCNTs for the detection of antibiotics in real effluents

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Commission : chimie

Salle : 2

Mots clés : f, MWCNTs, antibiotics and electrochemical detection

Abstract :

Antibiotics can accumulate through food metabolism in the human body which may have a considerable effect on human safety and health. It is therefore highly beneficial to establish easy and sensitive approaches for rapid assessment of antibiotic amounts. Carbon nanotubes are an interesting class of nanomaterial offering high electrical conductivity, high surface area, significant mechanical strength and good chemical stability, is increasingly used for sensitive and selective detection of antibiotics [1-3]. Sulfonamides are among the most commonly consumed antibiotics for both human health and veterinary applications. However, these compounds are among the priority pollutants to be monitored since they (i) have a high potential to resist degradation and (ii) are hydrophilic enough to be transferred into a wide variety of matrices such as waters, soils, crops, animal tissues, and bio-fluids [4]. The aim of this work is the preparation of a glassy carbon electrode (GCE) modified with carboxylic acid functionalized multi-walled carbon nanotubes (f-MWCNT) for the electrochemical determination of sulfamethoxazole (SMX) and ciprofloxacin (CIP) in three real effluents. The f-MWCNT/GCE was suggested here as a promising on-site detection tool for point-of-care monitoring of two antibiotics with simple and facile electrode preparation, rapid, sensitive, repeatable, and reproducible electrochemical responses.



JDD2023 :8-9 Mai 2023

Inhibition du tartre dans l'eau dure par des champs magnétiques

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Code : 469560

Commission : chimie

Salle : 2

Mots clés : entartrage, carbonate de calcium, champ magnétique, précipitation contrôlée rapide, méthode chronoampérométrique.

Abstract :

L'entartrage est l'un des problèmes indésirables de l'eau dure naturelle, qui entraîne d'énormes conséquences techniques et économiques par la formation de dépôts compacts et adhérents sur les canalisations et les installations industrielles ou domestiques. L'objet de cette étude était d'examiner les effets du traitement magnétique sur le pouvoir entartrant de l'eau dure en utilisant la précipitation rapide contrôlée (PCR) et la méthode chronoampérométrique (CA). L'influence de ce traitement sur la précipitation du carbonate de calcium a été confirmée. Ainsi, les résultats expérimentaux ont montré que l'augmentation du temps de magnétisation conduit à un retard dans la formation de CaCO_3 à la fois dans la solution et à la surface. Pour la méthode PCR, l'efficacité anti-tartre des aimants permanents appliqués était d'environ 60 % après 18 heures de traitement. Les résultats de CA ont montré que l'augmentation de l'intensité du champ magnétique de 0,33 T à 0,70 T contribue à une diminution du taux d'entartrage. Par conséquent, l'efficacité de l'inhibition passe de 65 % à 88 %. D'autre part, la morphologie des tartres minérales obtenues a été analysée par microscopie électronique à balayage (MEB) et caractérisée par diffraction des rayons X (DRX).



JDD2023 :8-9 Mai 2023

Synthesis, analysis, and molecular docking design of novel pyran-based Heterocyclic compounds

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Commission : chimie

Salle : 2

Mots clés : benzopyran, N, acyl hydrazone, anti, α , amylase, molecular docking

Abstract :

Over the last two decades, N-acyl hydrazone (NAH) has been proven to be a very versatile and promising motif in drug design and medicinal chemistry¹. In the light of these findings, and in the search for therapeutic alternatives to treat hyperglycemia, a series of twelve benzopyranic hydrazones 4a–l, was synthesized from the condensation reaction of benzopyran-hydrazide 3 (previously prepared from the corresponding 2-amino-3-cyanopyran 2) with a series of aryl aldehydes in ethanol. The synthesized compounds were characterized by spectroscopic means (¹H NMR, ¹³C NMR, HRMS) and their α -amylase inhibitory activity was predicted using molecular docking analysis. The simulation results highlighted the high binding affinity of compounds 4e, 4f, and 4k towards the α -amylase enzyme.



JDD2023 :8-9 Mai 2023

Geographical and Botanical Origin discrimination of Tunisian and Italian Honey using artificial senses

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Commission : chimie

Salle : 2

Mots clés : Honey, Geographical Origin, Botanical Origin, E, tongue, E, nose, E, eye

Abstract :

The need for a rapid and efficient aid decision tools is still growing thanks to their applications in many industries, particularly, in food production, for adulteration preventing, process monitoring and product quality control. In this frame, smell and taste sensors were developed. The design of these artificial or electronic noses and tongues is based on a new approach mimicking the mammalian olfaction and gustation. [1] In this work we used different artificial senses such as e-tongue, e-nose and e-eye for the discrimination between Tunisian and Italian honey. In fact, one of the most highly valued and consumed product is honey which can vary in its flavor and impact on human health depending on its geographical and botanical origin. [2-4] Our study was conducted using the Principal component analysis (PCA) method which proved that the e-tongue is the most efficient tool to use in order to discriminate between different types of origins of honey.