Book of Abstracts

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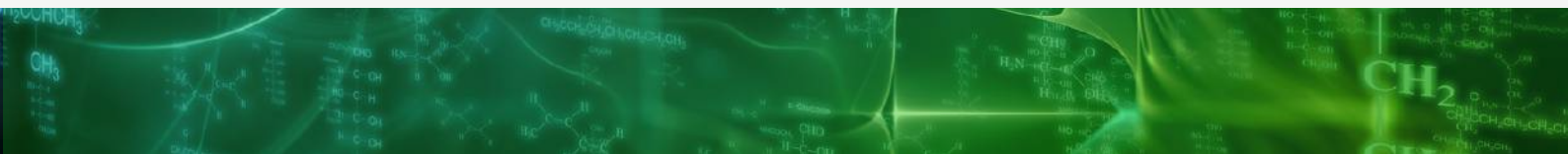

Contents

This book contains all abstracts submitted for the poster Session to the International UFAZ Conference, CPM's 2025 Edition.

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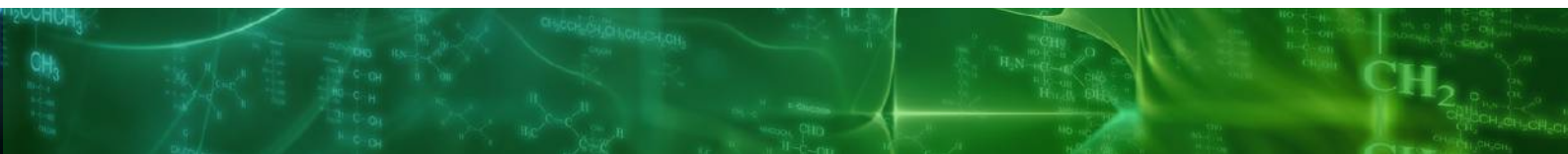

Abstracts

Comparative Analysis of the Antifungal Activity of α-Keto Acid Aril Hydrazone Derivatives

Shafiga Ibrahimova[1] , Gulnar Atakishiyeva[1] , Irada Shikhaliyeva[1] , Nigar Ahmadova[1] , Gulnara Babayeva[1,2] , Abel Maharramov[1]

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Abstract

In silico (computer-based) analyses were conducted to evaluate the possible antifungal activities of two different synthesized compounds – methyl (Z)-4-(2-methoxy-2-oxo-1-(2-(p-tolyl)hydrazineylidene)ethyl)benzoate and methyl (Z)-4-(1-(2-(3,4-dimethylphenyl)hydrazineylidene)-2-methoxy-2-oxoethyl)benzoate – against fungal pathogens. The results obtained through the PASS (Prediction of Activity Spectra for Substances) program were used to assess and compare the potential antifungal effects of these compounds against Galactomyces geotrichum and Epidermophyton floccosum species. For the first compound, PASS results indicated a 0.1781 probability of activity against Galactomyces geotrichum, suggesting that the compound might exhibit noticeable, though not strong, antifungal activity against this fungus. The predicted activity score for Epidermophyton floccosum was 0.1099, indicating weak, but not negligible, biological activity potential against this species. For the second compound, the activity score against Galactomyces geotrichum was slightly higher at 0.1824, indicating a slightly stronger antifungal potential compared to the first compound. However, the predicted activity against Epidermophyton floccosum was much weaker, with a score of 0.0608, indicating very limited antifungal effect against this pathogen. Overall, the results suggest that both compounds may exhibit significant antifungal activity against Galactomyces geotrichum, although their effect against Epidermophyton floccosum is weaker. Therefore, both compounds can be considered for further evaluation as potential antifungal agents. However, to determine their effectiveness and safety profiles more accurately, in vitro and in vivo experimental studies are required.

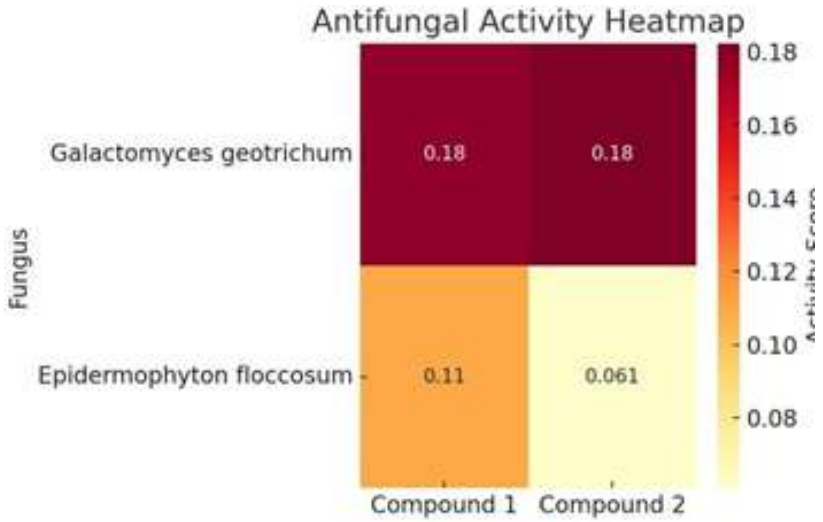

Fig. 1: Graph of the probability of antifungal activity of the compounds.

Graphical Analysis of Predicted Activity Against HIV-1 Target and Clinical Conditions Based on In Silico Analyses

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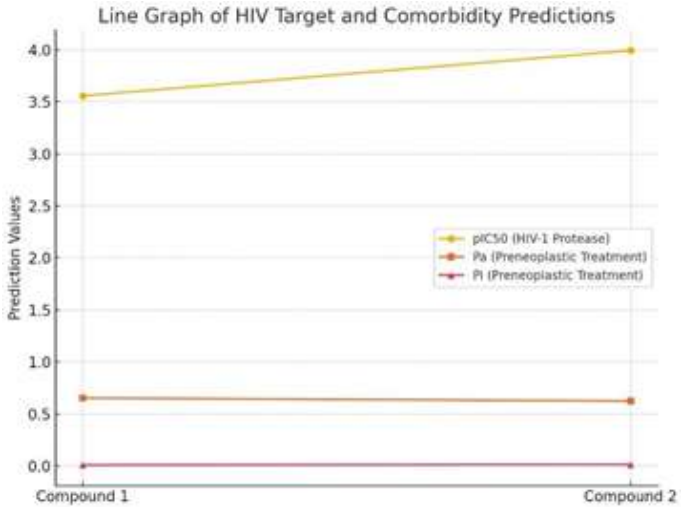
Abstract

In silico analyses conducted using the PASS program evaluated two synthesized compounds for their potential antiviral effects against the HIV-1 protease enzyme and their possible biological activity in the treatment of HIV-related preneoplastic conditions. The predicted results were analyzed both through numerical values and visual diagrams. The activity potential of both compounds against HIV-1 protease was expressed as pIC_{50} values. For the first compound, the pIC_{50} value was 3.558, and for the second compound, it was 3.994. These values indicate significant inhibitory effects, though they are not considered sufficiently high for strong antiviral activity. Since these results fall outside the application scope of the PASS model ("not in AD"), experimental validation is necessary to confirm their accuracy. On the other hand, the predicted activity for treating preneoplastic conditions related to HIV was more promising. The first compound showed a Pa (Probability of Activity) value of 0.654, while the second compound had a Pa of 0.625, both suggesting a high likelihood of biological activity. The Pi (Probability of Inactivity) values were very low, at 0.01 and 0.014, respectively, further reinforcing the reliability of the results



The visual graphs prepared for these analyses show that both compounds exhibit similar but weak effects against the HIV-1 protease target. In contrast, they demonstrate considerable activity in treating preneoplastic conditions. The linear graph and bar charts indicate that both compounds may be more promising for the treatment of HIV-related comorbid conditions rather than as direct antiviral agents

In Silico Blood Cancer Cell Line Cytotoxicity Analysis Of Two Hydrazone Derivatives Using BC CLC-Pred Tool

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Abstract

Hydrazone-based compounds have demonstrated diverse biological activities, including potential anticancer effects. In this study, two structurally related hydrazone derivatives — methyl (Z)-4-(2-methoxy-2-oxo-1-(2-(p-tolyl)hydrazineylidene)ethyl)benzoate (Compound 1) and methyl (Z)-4-(1-(2-(3,4-dimethylphenyl)hydrazineylidene)-2-methoxy-2-oxoethyl)benzoate (Compound 2) — were analyzed for cytotoxicity against human breast cancer cell lines using the BC CLC-Pred platform. Compound 1 showed predicted activity against MCF7-DOX and ZR-75-1 lines, with pGI50 values reaching 6.3780 in MX-1 and 5.7892 in MCF7R. On the other hand, Compound 2 demonstrated broader IC50-based activity, including Bcap37, MX-1, and ZR-75-1, with pGI50 values as high as 6.6076 (MX-1) and 6.7159 (ZR-75-1). Both compounds were inactive on Hs-578T and BT-20 lines, with minimal differences in pGI50 scores. These in silico insights suggest that structural variation at the hydrazone moiety influences selective cytotoxicity, with Compound 2 exhibiting stronger and more consistent responses in blood cancer-relevant cell models. Further in vitro validation is recommended.

Table 1. Cytotoxicity Prediction of Hydrazone Derivatives on Breast Cancer Cell Lines

Cell Line	Compound 1 - IC50	Compound 1 - pGI50	Compound 2 - IC50	Compound 2 - pGI50
Bcap37	inactive		active	5.6244
BT-20	inactive	5.6813	inactive	5.6244
Hs-578T	inactive		inactive	
MCF7		5.2556		5.2069
MCF7-DOX	active		inactive	
MCF7R	inactive	5.7892	inactive	
MX-1	inactive	6.3780	active	
T47D	inactive	5.1252	inactive	5.3181
ZR-75-1	active	5.4130	active	5.4923

Comparative In Silico Evaluation of Two Hydrazone Derivatives for Antiviral and Antitumor Potential

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Abstract

Hydrazone derivatives represent a versatile class of compounds with promising antiviral and antitumor activities. In this study, two novel compounds, methyl (Z)-4-(2-methoxy-2-oxo-1-(2-(p-tolyl)hydrazineylidene)ethyl)benzoate (Compound 1) and methyl (Z)-4-(1-(2-(3,4-dimethylphenyl)hydrazineylidene)-2-methoxy-2-oxoethyl)benzoate (Compound 2), were evaluated using two computational platforms: AntiVir-Pred and CLC-Pred. Compound 2 showed higher predicted activity against Dengue virus genome polyprotein (Pa = 0.7130), while Compound 1 demonstrated broader antiviral interactions, including SARS-CoV-2 and HIV-2. CLC-Pred results indicated that both compounds were potentially active against NCI-H838 (lung cancer) and HT-29 (colon cancer), with Compound 2 also targeting pancreatic carcinoma (YAPC). Non-tumor cell line HEK293 showed moderate sensitivity. These in silico results highlight both compounds as potential antiviral and anticancer candidates and warrant further experimental validation.

Table 1. Predicted antiviral activity (Pa values)

Target Virus / Protein	Compound 1 (Pa)	Compound 2 (Pa)
Dengue virus genome polyprotein	0.6761	0.7130
Vaccinia virus DNA polymerase	0.2666	0.2411
SARS-CoV-2 replicase polyprotein	0.1772	0.0672
HIV-2 integrase	0.1707	0.1371
Coxsackievirus B3 genome polyprotein	0.0954	0.0771
Infectious bronchitis virus 3C-like protease	0.0494	0.0350
Dengue virus NS3 protein	0.0416	0.0247
SARS coronavirus 3C-like proteinase	0.0136	0.0183

Table 2. Predicted cytotoxicity against cancer cell lines (Pa values)

Cell Line	Tissue	Tumor Type	Compound 1 (Pa)	Compound 2 (Pa)
NCI-H838	Lung	Carcinoma	0.393	0.441
HT-29	Colon	Adenocarcinoma	0.352	0.374
8505C	Thyroid	Carcinoma	0.313	0.315
CCRF-CEM	Blood	Leukemia	0.282	-
YAPC	Pancreas	Carcinoma	-	0.314

Table 3. Predicted cytotoxicity against non-tumor cell lines

Cell Line	Tissue	Compound 1 (Pa)	Compound 2 (Pa)
HEK293	Kidney	0.353	0.330
HEL 299	Lung	0.177	-

Droplet-Based Microfluidic Synthesis of MOFs: Fast Crystallization and Morphological Control

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Abstract

Metal-Organic Frameworks (MOFs) are a class of porous crystalline materials constructed from metal ions and organic ligands. Their large surface area, tunable porosity, and structural diversity [1] make them highly promising candidates for applications in gas storage, separation, catalysis, and drug delivery. [2] However, conventional methods of MOF synthesis, such as solvothermal or hydrothermal crystallization [3], are typically time-consuming and lack precise control over particle morphology. In this study, we present an accelerated and tunable method for MOF crystallization using a microfluidic approach based on a core-shell capillary system, which allows for faster synthesis and improved control over crystal structure and shape.

The synthesis was carried out using an aqueous solution of copper(II) sulfate ($CuSO_4$) as the core phase and a solution of benzene-1,3,5-tricarboxylic acid (also known as trimesic acid), neutralized with sodium hydroxide (NaOH), as the shell phase. These two precursor solutions were injected into a capillary microfluidic device in a core-shell configuration, and silicone oil was used as the continuous phase to generate isolated droplets containing the reacting species. The droplets were then passed through a polytetrafluoroethylene (PTFE) tubing, which was externally heated to temperatures ranging from 60 °C to 85 °C. This thermal environment facilitated rapid nucleation and growth of MOF crystals directly inside the droplets, eliminating the need for overnight incubation typically required in bulk synthesis. [4]

Additionally, to investigate the influence of solvents on crystal formation, we performed a series of experiments comparing water-based systems with those containing N,N-dimethylformamide (DMF). Notable differences were observed: in water, the resulting Cu-BTC MOF crystals displayed elongated, needle-like morphologies, and in some cases, complex star-shaped structures were formed. In contrast, the use of DMF led to the formation of smaller, more spherical crystals. These findings indicate that the choice of solvent plays a crucial role in tuning the final morphology of the MOFs and can be leveraged to customize them for specific applications.

Our approach demonstrates a significant reduction in synthesis time and offers morphological control that is difficult to achieve through conventional methods. The continuous-flow nature of the system also opens up possibilities for scaling up the production of MOFs in a controlled and reproducible manner. The rapid in-droplet crystallization enabled by the microfluidic platform is particularly advantageous for producing MOFs with properties tailored for biomedical uses, such as targeted drug delivery systems, where particle shape and size critically affect and biocompatibility.

This study proves that capillary microfluidics is a powerful tool for accelerating the synthesis of metal-organic frameworks while providing fine control over their structural properties, marking a step forward in the development of scalable and application-driven MOF fabrication technologies.

Keywords: Metal-Organic Frameworks (MOFs), Microfluidic synthesis

References

1. L. Jiao, J. Y. R. Seow, W. S. Skinner, Z. U. Wang, and H.-L. Jiang, “Metal–organic frameworks: Structures and functional applications,” Mater. Today, vol. 27, pp. 43–68, Jul. 2019, doi: 10.1016/j.mattod.2018.10.038.
2. U. Mueller, M. Schubert, F. Teich, H. Puetter, K. Schierle-Arndt, and J. Pastré, “Metal–organic frameworks—prospective industrial applications,” J Mater Chem, vol. 16, no. 7, pp. 626–636, 2006, doi: 10.1039/B511962F.
3. “How to Make Metal-Organic Frameworks (MOFs),” Ossila. Accessed: Apr. 15, 2025. [Online]. Available: https://www.ossila.com/pages/how-to-make-metal-organic-frameworks
4. A. Nowacka, P. Briantais, C. Prestipino, and F. X. Llabrés I Xamena, “Facile ‘Green’ Aqueous Synthesis of Mono- and Bimetallic Trimesate Metal–Organic Frameworks,” Cryst. Growth Des., vol. 19, no. 9, pp. 4981–4989, Sep. 2019, doi: 10.1021/acs.cgd.9b00237.

Antitarget Interaction Prediction Of Two Hydrazone Derivatives

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Abstract

In silico prediction of off-target interactions is crucial in early drug discovery to avoid adverse effects. This study evaluates the antitarget profiles of two hydrazone derivatives using the AntiTarget-Pred tool. Compound 1 (methyl (Z)-4-(2-methoxy-2-oxo1-(2-(p-tolyl)hydrazineylidene)ethyl)benzoate) and Compound 2 (methyl (Z)-4-(1-(2-(3,4-dimethylphenyl)hydrazineylidene)-2- methoxy-2-oxoethyl)benzoate) were analyzed for predicted interactions with undesirable targets. Compound 1 showed strong interactions with carbonic anhydrase I and II (pKi > 7.6), serotonin (5-HT2C) receptor (Ki = 6.650), and sodium-dependent transporters. Compound 2 revealed an even broader profile, interacting with 12 antitargets including 5-HT2C (Ki = 7.364), alpha1B-adrenergic receptor (Ki = 7.278), and carbonic anhydrase II (Ki = 7.627). Both compounds showed moderate to high binding probability to neurotransmitter transporters and dopamine/adrenergic systems, suggesting potential CNS-related offtarget effects. Most predictions fell within the applicability domain (AD), indicating reliable modeling output. These findings highlight the importance of structure-based profiling and provide insight into the safety risks associated with both compounds.

Table 1. Selected Antitarget Predictions for Compounds 1 and 2

Antitarget	Activity Type	Compound 1 - pKi/pIC50	Compound 2 - pKi/pIC50	Applicability Domain (AD)
5-HT2C receptor antagonist	Ki	6.650	7.364	In AD
Carbonic anhydrase II inhibitor	Ki	7.831	7.627	In AD
Carbonic anhydrase I activator	Kact	7.797	7.611	In AD
Amine oxidase A inhibitor	Ki	6.924	6.984	In AD
Alpha1B adrenergic receptor antagonist	Ki	7.094	7.278	In AD
Sodium-dependent serotonin transporter antagonist	Ki	7.082	7.221	Out of AD
Mu-type opioid receptor antagonist	IC50	5.972	5.898	In AD
Estrogen receptor antagonist	Ki	5.889	5.761	In AD

Prediction Of Metabolic Sites Of 1,1-Dichlorodiazabutadienes Synthesized Based On Methyl 4-Formylbenzoate

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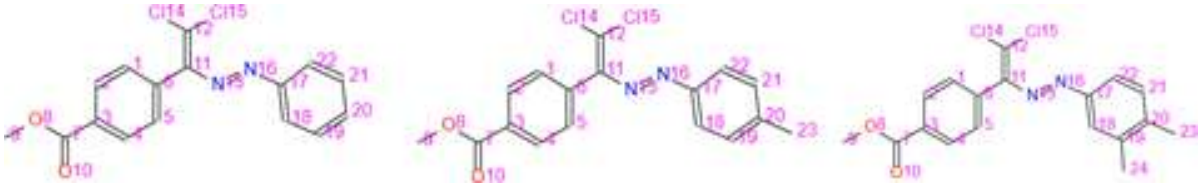
Abstract

SOMP (Site of Metabolism Prediction) is an approach used to predict the specific sites where pharmacological compounds undergo metabolism in the body. This method helps identify enzymatic degradation regions of drugs, allowing for the assessment of their metabolic stability and potential toxic metabolites. SOMP plays a crucial role in drug design by optimizing metabolic profiles and minimizing potential adverse effects. Considering this, we have predicted the metabolic sites of 1,1-dichlorodiazabutadienes synthesized based on methyl 4-formylbenzoate [1], and the results are presented in the following figures.



Compound I Compound II Compound III

For Compound I: To enhance the drug's metabolic stability, chemical modifications can be applied to atoms 9 and 20, which are highly metabolized by CYP3A4. This can be achieved by introducing steric hindrance or altering electron distribution. If the goal is to generate an active metabolite, regions with high metabolic activity (atoms 9, 20, and 19) can be considered. To reduce drug degradation, regions with low metabolic activity (such as atoms 1, 5, 2, and 4) should remain unchanged. For Compound II: To improve metabolic stability, chemical modifications can be applied to atoms 9 and 23, which are highly metabolized by CYP3A4. If the goal is to preserve the drug's active form, regions with low metabolic activity (such as atoms 1, 5, 2, and 4) should be left intact. If the aim is to generate active metabolites through metabolism, regions with high metabolic activity should be considered. For Compound III: To increase the drug's metabolic stability, chemical modifications can be applied to atoms 9, 23, and 24, which are highly metabolized by CYP3A4. If the objective is to maintain the active form of the drug, regions with low metabolic activity (such as atoms 1, 5, 2, and 4) should remain unchanged. To promote the formation of active metabolites, areas with high metabolic activity should be explored.

Keywords: Dichlorodiazadienes, site of metabolism prediction

References

1. N.Q.Shikhaliyev, S.A.İbrahimova, G.T.Atakishiyeva, N.E.Ahmedova, G.V. Babayeva, V.N. Khrustalev, Z.Atioğlu, M. Akkurt, and A. Bhattarai, Structure Reports, 2024, 80,2, 184-190.

DFT study of metal-polymer complex Cu–PVP

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Abstract

Selective oxidation of organic compounds holds significant theoretical and practical importance both in science and industry. The production of target products is also economically beneficial, as it allows for resource savings. In this context, the development and design of new catalysts remains highly relevant. A crucial aspect is the identification of the mechanisms underlying catalytic reactions. However, this introduces a new economic challenge: selecting optimal conditions and choosing the appropriate catalyst—including its synthesis—can require substantial time and resources. In such cases, computational modeling becomes a valuable tool. Computational chemistry has emerged as an essential instrument for investigating catalytic processes, both in homogeneous and heterogeneous phases. Characterizing reaction mechanisms using density functional theory (DFT) allows for a deeper understanding and optimization of the processes [1].

In the present work, quantum chemical calculations were performed using the Gaussian 09 program. DFT was chosen as the computational method, employing the B3LYP exchange-correlation functional with the 6-31G(d) and LANL2DZ basis sets. Geometry optimization was carried out for oligomer molecules of polyvinylpyrrolidone (PVP). Subsequently, after identifying the active sites, the structures of metal–polymer complexes (MPCs) of PVP monomer with copper were proposed and optimized. As a result of the calculations and analysis of the molecular electrostatic potential (MEP), it was revealed that the oxygen atom serves as the active site in the oligomer molecules. Based on the Mulliken charge values, the nitrogen atom shows a higher tendency to interact with the metal; however, due to steric hindrance, it does not participate in donor–acceptor or van der Waals interactions, which is also confirmed by the MEP surface. During the modeling of metal–oligomer complexes, metal atoms were placed near the oxygen atoms for structural optimization of the proposed complexes. The calculations yielded PVP monomer–Cu–PVP monomer complexes with a bond angle of 179.39° and O–Cu bond lengths of approximately 1.86 Å, indicating the formation of a coordination compound between copper and the polymer ligand. The bond energy is 420.08 kJ/mol, that indicates a strong coordination bond between Cu+ and the PVP ligand, further confirming the stability of the Cu/PVP complex.

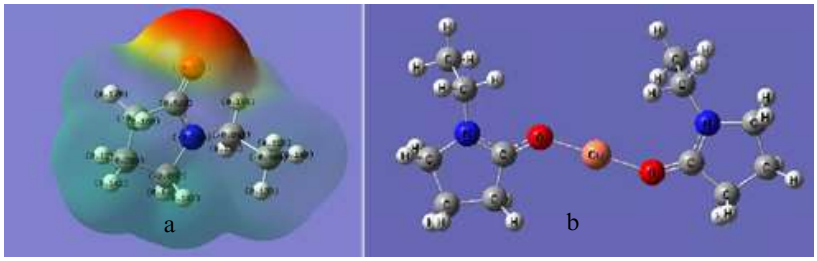

Fig. 1. Surface of MEP of the PVP monomer (a) and the structure of the obtained MPC of copper with the PVP monomer (b). Thus, computational chemistry, and in particular DFT studies, provide valuable insights into the structures of various compounds, the analysis of interactions between them, and the assessment of the likelihood of complex formation and their stability. The obtained molecules are planned to be used for modeling the adsorption of hexane, with the calculation of adsorption energy. In addition, the process of catalytic oxidation of hexane will be studied by finding the structure and energy of the activated complex.

Keywords: density functional theory (DFT), polyvinylpyrrolidone (PVP), metal–polymer complexes (MPCs), bond energy

References

1. Becke, A. D.: Perspective: Fifty years of density-functional theory in chemical physics. The Journal of Chemical Physics, 140(18), 18A301 (2014).

Thermodynamic properties of manganese indium selenide

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Abstract

Ternary chalcogenides based on transition metals of the AB2X4 type (where M = Mn, Fe, Co, Ni; B = Ga, In, Sb, Bi; X = S, Se, Te) are promising materials for the development of lasers, light modulators, photodetectors, and other functional devices controlled by magnetic fields. Some of these compounds are magnetic topological insulators, meaning they combine the properties of topological insulators and ferromagnets (or antiferromagnets). This makes them highly attractive for applications in spintronics, quantum computing, dark matter detectors, and more. Recent studies have also shown their potential in photocatalysis, photogalvanics, and thermoelectric converters [1–5]. Work presents the results of a comprehensive study of solid-phase equilibria in the Mn–In–Se system in the composition range MnSe–In_2Se_3–Se and the thermodynamic properties of the ternary compounds $MnIn_2Se_4$ and $Mn_2In_2Se_5$.

The studies used X-ray diffraction (XRD) and electromotive force (EMF) measurements. XRD of powder samples was performed using a "D2 Phaser" diffractometer (Bruker, Germany; CuKα radiation, 2θ range from 5° to 80°). To carry out the thermodynamic investigations, we assembled concentration cells of type (1) and measured their EMF in the temperature range of 300–450 K: (-) Mn (solid) | glycerin + KCl + $MnCl_2$ | (Mn in alloy) (solid) (+) (1) Measurements were performed using a digital voltmeter (Keihtley Model 193) with an input resistance of 10^{14} Ohms and an accuracy of ±0.1 mV and steps not exceeding 10 K. The temperature was monitored using chromel-alumel thermocouples and a mercury thermometer with an accuracy of 0.5 K. In type (1) cells, the electrolyte was a glycerin solution of KCl with the addition of MnCl2. MnSe was used as the left electrode, while various equilibrium alloys from different phase regions of the MnSe–In_2Se_3–Se subsystem were used as the right electrodes. The MnSe compound and alloy electrodes were synthesized by direct reaction of high-purity elemental components in evacuated (10^{-2} Pa) quartz ampoules at 1400 K, followed by homogenizing annealing at 900 K (500 h), and then at 450 K (200 h). Based on XRD data and literature sources, solid-phase equilibrium diagrams of the MnSe– In_2Se_3–Se system were constructed. It is shown that the system forms ternary compounds $MnIn_2Se_4$ and $Mn_2In_2Se_5$, which form stable connod with elemental selenium. The partial thermodynamic functions of Mn in the alloys were determined from the EMF measurements of concentration chains of type [1] in the phase regions $MnIn_2Se_4$- In_2Se_3- Se and $Mn_2In_2Se_5$- $MnIn_2Se_4$-Se, on the basis of which the standard thermodynamic functions of formation and standard entropies of compounds $MnIn_2Se_4$ and $Mn_2In_2Se_5$ were calculated using literature data on the thermodynamic properties of In_2Se_3.

References

1. K. Guratinder, M. Schmidt, H. C. Walker et.al. Magnetic correlations in the triangular antiferromagnet FeGa2S4. Phys. Rev. B. 104(6), 064412 (2021).
2. Yang J., Zhou Z., Fang J. et.al. Magnetic and transport properties of a ferromagnetic layered semiconductor MnIn2Se4. Appl. Phys. Lett. 115(22), 222101 (2019).
3. D. A. Estyunin, I. I. Klimovskikh, A. M. Shikin et.al. Signatures of temperature driven antiferromagnetic transition in the electronic structure of topological insulator MnBi2Te4, APL Mater. 8(6), 021105 (2020).
4. P. Wyz˙ga, I. Veremchuk, M. Bobnar et.al. Ternary MIn2S4 (M = Mn, Fe, Co, Ni) Thiospinels – Crystal Structure and Thermoelectric Properties. Z. Anorg. Allg. Chem. 646(14), 1091 (2020).
5. H. Liang, T. Feng, S. Tan et.al. Two-dimensional (2D) MnIn2Se4 nanosheets with porous structure: a novel photocatalyst for water splitting without sacrificial agents. Chem. Commun. 55, 15061(2019).

Photoelectrochemical water splitting and photocatalytic decomposition performance of visible light active MgMnO3 perovskite nanostructure

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Abstract

Sustainable and clean energy sources coupled with ecological rehabilitation rank as top priorities for achieving robust sustainability objectives. There is a pressing need for multifunctional materials that can effectively tackle both concerns, driving high demand in scientific communities. In this study, a photoactive magnesium manganese oxide (MgMnO3) perovskite nanoarchitecture was developed through a simple citrate sol–gel technique for the photocatalytic disintegration of ciprofloxacin (CIP) antibiotic and methylene blue (MB) dye, alongside photoelectrochemical (PEC) water splitting. The MgMnO3 nanomaterial was investigated via a multifaceted approach employing XRD, FESEM, XPS, PL, EDX, and UV-Vis spectrophotometer to uncover its intrinsic physiochemical and optoelectronic attributes. The MgMnO3 catalyst attained maximal performance of 88% and 96% for photodecomposition of CIP (10 mg/L) and MB (10 mg/L), respectively, using 35 mg and 30 mg of catalyst quantity over 90 minutes. The MgMnO3 electrode showcases superior photoelectrochemical behavior, with a maximal photocurrent density of 13.21 mA cm-2 measured at 1.2 V vs. RHE and achieving a solar-to-hydrogen conversion efficiency of 2.45% compared to MgO and MnO2 photoelectrode. Notably, the MgMnO3 electrode reveals outstanding photoelectrochemical durability, maintaining its stability even after continuous illumination for 9 hrs. This impressive photoelectrochemical ability arises from the wider range of light absorption, improved carrier separation, and more successful transfer and utilization mechanisms. This study introduces a pioneering approach for the fabrication of efficient and enduring multifunctional catalysts, catering to both photocatalytic degradation and photoelectrochemical (PEC) characteristics essential for hydrogen generation.

Keywords: Metal-organic framework, carbon capture and conversion, climate change

References

1. Prabagar JS, Tenzin T, Sneha Y, Divya V, Anusha HS, Shahmoradi B, et al. Novel NiFeAl hybridized layered double hydroxide nanofibrous for photocatalytic degradation and CO_2 reduction. Materials Today Sustainability 2024;26:100773.
2. Jiang W, An Y, Wang Z, Wang M, Bao X, Zheng L, et al. Stress-induced $BiVO_4$ photoanode for enhanced photoelectrochemical performance. Appl Catal B Environ 2022;304:121012

Determination of the Properties of Polymer-supported Nickel Nanocatalyst by DLS Method

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Abstract

Particle size is one of the key parameters for supported metal catalysts, as it significantly affects their activity and selectivity. Determining particle size is an essential task, and the development of cost-effective, sensitive, and simple methods remains a relevant research focus. Dynamic Light Scattering (DLS) is considered a fast and inexpensive method for particle size determination [1,2].

For this purpose, a polymer/metal-based complex was synthesized and the average particle size was determined using a DLS device. First, a gelatin and poly-N-vinylpyrrolidone copolymer was synthesized. Nickel metal was immobilized on the copolymer for use as a catalyst. To ensure the sustainability of the acquired complex, a croslink process was carried out with a crosslinking agent [3]. Results: The DLS device performs measurements within the range of 0.001–6 microns. The diffusion coefficient is calculated using the Stokes-Einstein equation [4]. The radiation source has a power of 5 mW and a wavelength of 650 nm. This method is based on recording fluctuations in the intensity of scattered light and measuring the average diffusion velocity of dispersed particles.The fluctuations in the intensity of scattered light, caused by the Brownian motion of particles, are characterized by the time-dependent autocorrelation function of the scattering intensity. The relaxation time of this function, up to its average value, is related to the properties of Brownian diffusion and directly measures the diffusion coefficient of particles in a liquid.Since the diffusion coefficient is functionally related to particle size, the DLS method also determines the size of these particles.

The analysis results provide the following measurements: the median nanoparticle size (nm), the mean value of the distribution density (nm), the mode representing the maximum particle size in the distribution curve (nm), and the calculated diffusion coefficient (m^2/sec). These values are presented in Table 1.

Table 1.

The name of instance	Median, nm	Mean, nm	Mode, nm	Diffusion Coefficient m^2/sec
Gelatin+PVP+Ni(10%)	7.5	7.5	7.2	3.4757E-11

Keywords: supported metal catalysts, particle size, DLS method.

References

1. Tuo, YX.(2018).Insight into the support effect on the particle size effect of Pt/C catalysts in dehydrogenation.J Catal 360:175–186.
2.Yu.V.Larichev (2021).Application of DLS for metal nanoparticle size determination in supported catalysts.Chemical Papers 75:2059–2066.
3.Rahimli N.Immobilization of Ni metal to PVP/Gelatin copolymer and investigation of its structure.EUCHEMBIOJ 2024: I. International Conference on Chemistry and Biotechnology,December 09, 2024, Istanbul,Türkiye.
4.Larichev Yu. V.(2021)//Application of DLS for metal nanoparticle size determination in supported catalysts//Chemical Papers,75:2059–2066. https://doi.org/10.1007/s11696-020-01454-1

Computer Modeling of Catalytic Systems Based on Metal-polymer Nanocomposites

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Abstract

Computational modeling techniques serve as indispensable instruments across contemporary chemistry, physics, and biology, as well as interdisciplinary domains. Density Functional Theory (DFT) is a computational modeling method extensively utilized in quantum chemistry and condensed matter physics. It serves as a powerful modeling technique for analyzing the electronic structure of atoms, molecules, and materials. The use of new technologies in chemistry allows to reduce the number of experiments, save resources, comparing the results of modeling with experimental data. These methodologies enable predictive insights into complex systems, driving innovation in materials science, drug discovery, and catalysis [1].

In this work, metal-polymer nanocomposites cobalt-polyvinylpyrrolidone (Co-PVP) were synthesized.The considered complexes were studied using quantum-chemical methods of analysis, in particular the density functional theory (DFT) method, which is a method for calculating the electronic structure of multiparticle systems in quantum physics and quantum chemistry. The calculations were performed using the Gaussian 09 program. The 6-31G and LANL2DZ basis sets were also used for calculation. For starting, we analyzed the PVP-Co system using DFT method to predict the nanocomposite structure, properties, and stability. This approach allows us to identify key interactions within the system and determine the dominant forces governing its behavior. As known [2-3], metal-polymer systems exhibit van der Waals forces, electrostatic interactions, donor-acceptor interactions, and, in some cases, hydrogen bonding.

Based on the calculations, we identified the structure of the complexes, active centers of molecules and the types of interactions, as well as the stability of the obtained complexes. It should be noted that the Co-PVP nanocomposites are quite stable, and electrostatic interactions between cobalt nanoparticles and PVP fragments are expected in the system. In addition, PVP serves as both a stabilizer, maintaining the size of the nanoparticles, and a matrix, preventing their aggregation. Based on the IR spectra of the obtained samples, the expected structure of the complexes was confirmed. There is a strong agreement between experimental and theoretical results. Thus, computer modeling is a powerful tool for the development of new materials and processes. It opens new horizons for research in chemistry and materials science, enabling more efficient and precise design of new materials, in particular catalysts for various industrial applications. With the development of computing technologies and analysis methods, this direction will continue to develop, offering new solutions for current scientific and technological problems.

Keywords: Computer modeling, DFT (density functional theory), cobalt-polyvinylpyrrolidone (Co-PVP).

References

1. S.S. Batsanov. Structural chemistry. facts and dependencies. – M: Dialogue-MSU, 2000- 335-347 p.
2. S. Yadav, N. Rani, K. Saini, A review on transition metal oxides based nanocomposites, their synthesis techniques, different morphologies and potential applications, IOP Conf. Ser.: Mater. Sci. Eng. 1225 (2022), 012004.
3. S.B. Singh, P.K. Tandon, Catalysis: A Brief Review on Nano-Catalyst, J. Energy Chem. Eng. 2 (2014) 103–112

Studying the Physical-mechanical Properties of Metal-carbon Nanocomposites Based on Low-pressure Polyethylene

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Abstract

The development of nanotechnology opens up new opportunities for extensive research in the field of composite materials. Currently, nanocomposite materials are used as promising polymeric materials that can be used in various fields of electronics [1].

The presented work is devoted to the preparation and study of the properties of nanocomposites based on high density polyethylene (HDPE) using cobalt oxide nanoparticles (NPCoO) stabilized by a polymer matrix and multi-walled carbon nanotubes (MWCNTs) as nanofillers. Physical-mechanical properties of the obtained nanocomposites were studied. The optimal ratio of nanocomposite samples was found.

Composition formulation (wt.%.)	Tensile strength, (σ_p), MPa	Specific elongation (ε_p), %	Vicat softening point, °C
HDPE (100)	25.41	440	130
HDPE/CoONP(100/0.5)	29.44	284	135
HDPE/CoONP (100/1.0)	31.22	350	140
HDPE/CoONP (100/2.0)	30.91	272	135
HDPE/MWCNT(100/0.01)	31.81	220	137
HDPE/MWCNT (100/0.05)	33.80	220	140
HDPE/MWCNT (100/0.1)	29.70	210	135
HDPE/CoONP /MWCNT (100/1.0/0.05)	32.59	400	145

As shown in Table , the introduction of 1.0% by weight of CoONPs into the composition of HDPE leads to an increase in the tensile strength from 25.41 to 31.22 MPa and the strain at break from 440 to 350%.

The results also show the effect of MWCNT on the physical-mechanical parameters of the nanocomposite: an increase in tensile strength from 25.41 to 33.80 MPa, with a decrease in elongation from 440 to 220%. At the same time, the Wicat softening point increases by 10 °C and a slight decrease in the crystallinity of the nanocomposite is observed. The combined use of CoONPs and MWCNT in a HDPE composite leads to an increase in the tensile strength index from 25.41 to 32.59 MPa while maintaining the elongation. The combined use of CoONPs and MWCNT in HDPE composite obviously overcomes the low compatibility of MWCNT with the polymer, which contributes to obtaining a composite with the best properties. A necessary condition for obtaining the best properties of carbon nanomaterials in a polymer composite is achieving the maximum degree of dispersion of the filler and its optimal orientation in the polymer matrix

Keywords: Cobalt-containing nanoparticles, Multilayer carbon nanotube, Metal carbon nanocomposites

References

1. Cubin S.P., Yurkov G.Yu., Kosobudsky I.D. Nanomaterials based on metal-containing nanoparticles in polyethylene and other carbon-chain polimers. International Journal of Materials and Product Technology 23(1 – 2), 2– 25 (2005).

Synthesis and Investigation of the Electrocatalytic Properties of Ni-P Thin Films

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Abstract

This study focuses on the electrochemical synthesis of nickel phosphide and the investigation of its electrocatalytic properties in neutral and alkaline media for the hydrogen evolution reaction (HER). An electrolyte and electrolysis conditions were developed for the synthesis of Ni-P thin films with electrocatalytic properties. $NiCl_2 \cdot 6H_2O$ and NaH_2PO_4 were used as precursors. The deposited film was found to consist of NiP_3 and Ni, with a phosphorus content of approximately 74 at.%. The high phosphorus content contributes to the enhanced electrocatalytic activity and corrosion resistance of the Ni-P thin films. The films exhibited high electrocatalytic activity for HER in an alkaline medium, with a Tafel slope of 135 mV/dec.

Water electrolysis is a key technological component in the development of a sustainable hydrogen economy. The electrocatalytic activity of electrodes in the hydrogen evolution reaction (HER) is a critical step in this process and has been extensively studied. Hydrogen is a clean alternative to fossil fuels, as its combustion produces only water as a byproduct and helps mitigate the intermittency of renewable energy sources. Ideally, H_2 should be produced via carbon-free pathways using solely renewable energy and resources. Transition metal-based compounds have emerged as promising and cost-effective alternatives to platinum, the most efficient HER electrocatalyst. Among them, nickel phosphides (Ni xPy) have garnered significant attention due to their remarkable HER activity. Nickel-rich NixPy can be viewed as Ni doped with P in its metallic lattice. Phosphorus-rich phases, NiP_2 and NiP_3, remain largely unexplored.

The kinetics and mechanism of nickel-phosphorus co-deposition were investigated using cyclic and linear polarization curves recorded with an IVIUMSTAT Electrochemical Interface potentiostat. To determine the elemental composition and electrocatalytic properties, Ni-P thin films were electrodeposited under galvanostatic conditions in a two-electrode cell on copper substrates at current densities of 20–30 mA/cm² for 0.5 hours at 338 K, with a platinum plate as the anode. Prior to deposition, copper substrates were cleaned in diluted HNO_3 (1:1) and degreased with ethanol and acetone. The asdeposited films were amorphous and subsequently annealed in an argon atmosphere at 673 K for 1 hour. Surface morphology was analyzed using a scanning electron microscope (SEM, Oxford Instruments), elemental composition was determined by EDX, and structural characterization was performed using a Rigaku Miniflex-500 X-ray diffractometer with CuKα radiation (λ = 1.54 Å).

To investigate the mechanism of co-deposition, cyclic and linear polarization curves were recorded for the co-deposition of nickel and phosphorus. Cyclic polarization measurements established the potential range for co-deposition and identified the anodic potentials at which the oxidation of the deposited compounds occurs. The Ni-P thin films obtained via galvanostatic deposition were amorphous and were subsequently annealed at 673 K for 1 hour to study their phase composition. X-ray phase analysis revealed that the NiP_3 deposits exhibited a trigonal symmetry, where phosphorus atoms formed a three-dimensional network and nickel atoms occupied specific positions, forming bonds with phosphorus atoms. This structure determines key properties, including mechanical strength, thermal stability, and electrocatalytic activity. To evaluate the electrocatalytic activity, linear polarization curves were recorded in an alkaline (1 M KOH) medium, and Tafel plots were constructed.

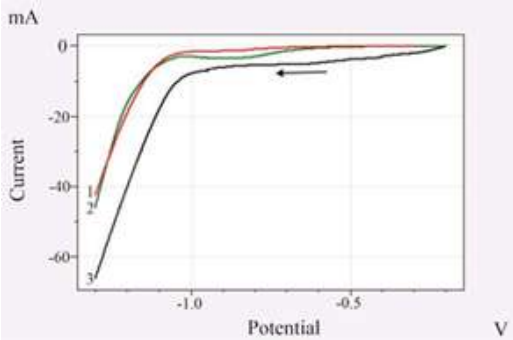

Fig. Electrocatalytic activity of electrodes for HER: 1 – NiP_3; 2 – St-3; 3 – Ni.

The electrocatalytic activity of NiP_3 exceeded that of electrodes traditionally used in industry (nickel, steel) for hydrogen production, with a Tafel slope of 135 mV/dec.

Ni-P thin films were successfully obtained via electrochemical deposition from an acidic electrolyte. X-ray phase analysis confirmed that the deposited film consists of NiP_3 and Ni, exhibiting a trigonal symmetry structure that influences its mechanical and electrocatalytic properties. The investigation of the electrocatalytic performance of NiP_3 thin films in an alkaline medium demonstrated that their catalytic activity surpasses that of electrodes traditionally used in industrial hydrogen production.

Keywords: electrodeposition, electrocatalysis, nickel-phosphorus.

References

1. Burchardt T., The hydrogen evolution reaction on NiPx alloys, International Journal of Hydrogen Energy, 25 (7), 627-634 (2000) https://doi.org/10.1016/S0360-3199(99)00089-0

2. Putri L. K., Ng B.-J., Yeo R. Y. Z., Ong W.-J., Mohamed A. R., Chai S.-P., Engineering nickel phosphides for electrocatalytic hydrogen evolution: A doping perspective, Chemical Engineering Journal, 461, 141845, (2023) https://doi.org/10.1016/j.cej.2023.141845

3. Morales-Guio C. G., Hu X., Amorphous molybdenum sulfides as hydrogen evolution catalysts, Accounts of Chemical Research, 47 (8), 2671-2681, (2014) https://doi.org/10.1021/ar5002022

Preparation of Nanoparticle Cooligomer-based Coatings in the Protection of Equipment from Corrosion in the Process of Biocorrosion

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Abstract

Biocorrosion is a process that occurs due to the impact of microorganisms on metal in various environments. This phenomenon arises from two primary causes:
- Microorganisms can serve as a nutrient source for the metal coating.
- The chemical compounds produced by microbial activity can accelerate corrosion.

Corrosion may occur across the entire metal surface or spread from one localized area to another. In cases where high-speed fluid flow interacts with the metal surface, corrosion progresses more aggressively, potentially leading to deep structural damage and operational failures. Given the diverse and hazardous nature of corrosion, consistent monitoring is essential due to its adverse economic effects. The presence of different types of microorganisms in the environment fosters biological film formation, contributing to biocorrosion. Protecting industrial equipment from such corrosion remains a key area of research.

Introduction
Biocorrosion is a critical issue in industrial settings, where nearly 2,500 different microorganisms contribute to the degradation of metal surfaces. The primary agents of this process are bacteria, which rapidly multiply and form biofilms. Water oxidation levels serve as an indicator of biofilm formation, as increased oxidation suggests higher contamination by organic matter. This process intensifies localized corrosion and weakens the material. Studies reveal that aggressive biofilms in seawater-based cooling systems significantly accelerate equipment deterioration. The uneven distribution of biological layers leads to electrochemical corrosion, further reducing the operational lifespan of metal structures.

Methods
This study focuses on developing a nanocomposite cooligomer-based protective coating to mitigate biocorrosion. The methodology involves the synthesis of nanocomposite coatings, surface adhesion analysis, and corrosion resistance evaluation. Laboratory experiments were conducted to assess coating effectiveness, including adhesion strength tests and exposure to corrosive environments. Comparative studies were performed to determine the efficiency of the proposed coating in reducing metal degradation.

Results
Experimental findings demonstrate that the nanocomposite cooligomer coating significantly enhances corrosion resistance. The results indicate superior adhesion to metal surfaces, ensuring prolonged protection. Additionally, the presence of nanoparticles improves structural integrity, reducing the impact of microbial activity on metal degradation. Comparative analysis with conventional coatings confirms that nanocomposite coatings provide greater durability and longer service life. Industrial trials suggest that applying these coatings can lead to considerable cost savings by minimizing equipment replacement and maintenance expenses. Moreover, the environmental benefits of reduced metal wastage highlight the broader implications of this technology.

Conclusion
The study confirms that nanocomposite cooligomer coatings effectively reduce biocorrosion effects, enhancing metal surface protection. This innovative solution not only extends equipment lifespan but also offers economic and environmental benefits. The findings suggest that adopting such coatings in industrial applications can significantly improve material performance, ultimately reducing maintenance costs and ensuring sustainable industrial operations.

Keywords: microorganisms, bacteria, biocorrosion, cooligomer, nanoparticles, coating

References

1. Knop A., Scheib W. Chemistry and Application of Phenolic Resins. New York. 1979, 272 p.
2. Qarayev S.F., Bilalov Y.M., Naibova T.M., Talıbov G.M. Chemical Resistant Composition for Coatings. Patent AR, I 2010 0062. 14.07.2010.
3. Beech I.B., Sunner J. Biocorrosion: towards understanding interactions between biofilms and metals. Current Opinion in Biotechnology. 2004;15(3):181-186.
4. Jeffrey R., Melchers R. The changing nature of microbiologically influenced corrosion. Corrosion Science. 2014;86:17-34.
5. Website: Corrosionpedia. "Understanding Microbiologically Influenced Corrosion (MIC)". Available at: https://www.corrosionpedia.com/ Accessed 2025/02/19

Comparative Analysis of the Effect of the Quaternization Process on the Electronic Structure of 4-vinylpyridine Oligomers (n=1-3) Using DFT Calculations

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Abstract

Due to their high thermal and chemical stability, 4-vinylpyridine oligomers are very important in various industrial applications. Thus, they are widely used in synthesizing functional materials in polymer chemistry, creating drug delivery systems, and in various chemical sensors. Also, the presence of the pyridine ring makes them very useful in catalytic studies. Considering all this, the study of 4- vinylpyridine oligomers is significant [1].

In this study, a comparative study of the structural and electronic properties of 4-vinylpyridine monomers and oligomers (n=2-3), as well as their quaternized (4-VP$^+$) analogs, was conducted based on Density Functional Theory (DFT). The effects of oligomer chain length and quaternization on HOMO-LUMO energy levels, charge distribution, electronic conductivity, and solvent effects were studied.

All quantum-chemical calculations were performed using the Gaussian09 software package. The structural and electronic properties of oligomers of 4-vinylpyridine and its methyl-quaternized analogs (n=2,3) were comparatively analyzed. Initial structures were prepared using GaussView 16.0 software. Based on literature reviews, the B3LYP hybrid functional and the 6-31G(d,p) basis set were selected. This combination is more useful for aromatic systems, as it gives reliable results and is optimal in terms of computational efficiency [2].

The structure of the molecule is schematically shown in Figure 1. Compounds 1,3,5 represent monomer, dimer, and trimer molecules, and 2,4,6 represent the corresponding quaternized molecules. The calculation results are summarized in Table 1. As we can see from the table, quaternization significantly reduces the HOMO-LUMO energy gap (ΔEgap) for the corresponding molecules. This decrease indicates that quaternized oligomers have higher electron conductivity. The decrease in electron affinity and ionization potential as a result of quaternization indicates an increase in electron density in the molecule and an improvement in the nucleophilic of the system. The decrease in hardness and electronegativity coefficients after quaternization indicates that the electron cloud of the molecule becomes softer and more deformable. A decrease in rigidity indicates a more free movement of electrons and an increase in the polarizability of the molecule, which leads to a more effective coordination ability with transition metal complexes. A decrease in the electronegativity coefficient characterizes a weakening of the electron acceptor property of the molecule and a strengthening of the electron donor property.

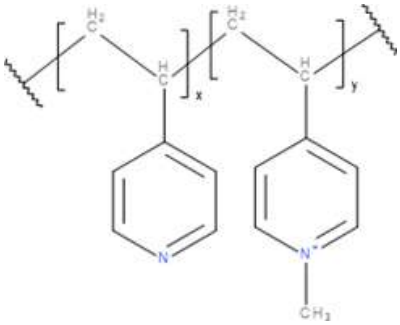

Figure 1. The structural scheme of compounds
Compound 1. x=1; y=0. Compound 2. x=0, y=1; Compound 3. x=2; y=0.
Compound 4. x=1; y=1. Compound 5. x=3; y=0. Compound 6. x=2; y=1

Table 1.

Compounds	EΔ, eV	IP, eV	EA, eV	η	χ
1	5,34	6,73	1,39	2,67	4,06
2	3,94	4,39	0,45	1,97	2,42
3	6,08	6,87	0,79	3,04	3,83
4	4,24	4,72	0,48	2,12	2,60
5	5,96	6,72	0,75	2,98	3,74
6	4,07	4,66	0,59	2,04	2,62

This study provides valuable information for the rational design and optimization of 4-vinylpyridine□based materials, especially those used in applications such as electroactive polymers, electrolyte membranes, and sensor materials. By varying the degree of quaternization, it is possible to tune the electronic and optical properties of the materials. Future studies will focus on modeling 4-vinylpyridine oligomers modified with different quaternization agents and further investigating the effect of the degree of quaternization on the oligomer properties.

Keywords: Quantum-chemical calculations, Density Functional Theory, Poly-4-vinylpyridine.

References

1. El-Hassan, A., & Amin, M. A. (2017). Synthesis and characterization of oligomer 4-vinylpyridine as a corrosion inhibitor for mild steel in CO_2-saturated brine solution. Indonesian Journal of Chemistry, 16(2):198, https://doi.org/10.13140/RG.2.2.31498.012

2. Zhao, H., Zhou, J., Hu, L., & Teng, Q. (2009). Theoretical Studies on Electronic Structures and NMR Spectra of Oligo(4-vinylpyridine). Chinese Journal of Chemistry, 27(9), 1687–1691. doi:10.1002/cjoc.200990283

The Role of the Initiator in the Synthesis of Acrylamide and Gum Arabic Graft Copolymer

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Abstract

In recent decades, the synthesis of biocompatible, naturally degradable, and absorbable new hydrogels for medical applications has been one of the most extensively researched fields. The increasing demand for these hydrogels emphasizes the importance of optimizing conditions, selecting the appropriate environment, initiator, crosslinking agent, and, in short, accurately defining the entire system for the synthesis of modified graft copolymers [1]. The aim of our study is to determine a suitable carrier system for the synthesis of gum arabic and acrylamide graft copolymer for the delivery of the Arbidol drug.

Based on this, the both syntheses were carried out at 70°C for a 2 hours by using azobisisobutyronitrile (AIBN) and ammonium persulfate (APS) initiators at different concentrations of the crosslinking agent [2-4]. Initial and the obtained products were analyzed using FTIR, XRD, and SEM methods. Additionally,the swelling degree of crosslinked GA-AM copolymers was also studied in aqueous and with different pH solutions [5,6]. Results: In the synthesis process with AIBN,copolymerization was observed to begin one hour after the addition of the crosslinking agent to the system, whereas with APS, it started after three minutes.This indicates that the APS initiator facilitates the conversion of numerous functional groups in the main chain polymer into free radicals, resulting in an easier bonding process between the polymer and the monomer. Based on the SEM analysis, the surface morphology of pure GA is rough and wavy, while the surface of the obtained hydrogel has smooth edges. Therefore, this indicates that the grafting reaction occurred efficiently.The grafting efficiency has been calculated based on this formula GE%=M(cop)-M(pol)/M(monomer) [7].

We analyzed and compared the outcomes of both syntheses, exploring the effect of the initiator on gel performance. The properties examined included gelation time, gel strength, swelling ratio. Based on the results, the use of APS as an initiator is considered more suitable for the synthesis of the copolymer.

Keywords: Gum arabic,acrylamide,grafting,initiator,copolymer.

References

1. Irina N. Savina, Bo Mattiasson,Igor Yu. Galaev//Graft Polymerization of Vinyl Monomers Inside Macroporous Polyacrylamide Gel, Cryogel, in Aqueous and Aqueous-Organic Media Initiated by Diperiodatocuprate(III) Complexes//Inc. J Polym Sci Part A: Polym Chem 44: 1952–1963, 2006// https://doi.org/10.1002/pola.21305

2.Róisín Holmes,Xue-Bin Yang,Aishling Dunne,Larisa Florea,David Wood and Giuseppe Tronci//Thiol-Ene Photo-Click Collagen-PEG Hydrogels: Impact of Water-Soluble Photoinitiators on Cell Viability, Gelation Kinetics and Rheological Properties//Polymers 2017, 9(6), 226; https://doi.org/10.3390/polym9060226

3.Graeme Moad//A Critical Assessment of the Kinetics and Mechanism of Initiation of Radical Polymerization with Commercially Available Dialkyldiazene Initiators//Progress in Polymer Science 2019,Vol.88, P.130-188 https://doi.org/10.1016/j.progpolymsci.2018.08.003

4.Yashu Chen//Characterization of free-radical solution polymerizations of acrylamide initiated by persulfate initiator systems//Missouri University of Science and Technology 2018,pages 59-69.

5.Yuwen Zeng,Pavlo Gordiichuk,Takeo Ichihara,Ge Zhang//An Irreversible Synthetic Route to an Ultra-Strong Two-Dimensional Polymer//Materials Science 2021.//DOI:10.48550/arXiv.2103.13925

6.Yujia Wang, Wenjie Song,Lijun Bao,Junwu Wei, Yangyang Qian and Yunmei Bi//Enzyme and pH dual responsive linear-dendritic block copolymer micelles based on a phenylalanyl–lysine motif and peripherally ketal-functionalized dendron as potential drug carriers// RSC Adv., 2023,13, 22079-2208

7.DOI: 10.1039/d3ra03790h 7.Marwa Aly Ahmed,Júlia Erdőssy,Viola Horváth//The Role of the Initiator System in the Synthesis of Acidic Multifunctional Nanoparticles Designed for Molecular Imprinting of Proteins/Periodica Polytechnica Chemical Engineering,2021,Vol. 65 No. 1 https://doi.org/10.3311/PPch.15414

Use of Microorganisms, Algae and Vermiculture for Bioremediation of Oil-Contaminated Sea Water

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Abstract

Oil pollution of marine ecosystems remains one of the most pressing environmental problems, especially in areas with intensive oil production. Bioremediation, using living organisms to decompose hydrocarbons, is considered one of the possible solutions. This paper compares the effectiveness of three bioremediation approaches: hydrocarbon-oxidising microorganisms, algae and vermiculture. Microorganisms isolated from oil-contaminated seawater are able to rapidly degrade hydrocarbons, algae (Laurencia caspica and Phaeophyceae) promote their sorption and release of oxygen, and vermiculture based on zoohumus obtained as a result of processing of organic wastes by larvae of the black lion fly (Hermetia illucens) can stimulate microbiological processes of oil decomposition. A comparison of these methods will identify the most effective strategies for cleaning seawater from oil contamination [1,2].

The experiment was conducted under laboratory conditions using oil-contaminated seawater. Oil from the Bibi-Eybat field was used as a pollutant. Four groups of samples were subjected to different treatment conditions: control group without exposure, treatment with hydrocarbon-oxidising microorganisms isolated from oil-contaminated seawater, exposure to algae (Laurencia caspica and Phaeophyceae), use of vermiculture based on zoohumus produced by processing by Hermetia illucens larvae. 100 ml of Mills' medium and 1 g of oil were added to each experimental container. Incubation was carried out at 28-30°C for 7 days. The decomposition efficiency of petroleum hydrocarbons was evaluated by gravimetric analysis after the filtration of samples.

At the end of the experiment, it was found that the efficiency of bioremediation methods varied. The highest oil degradation rates were observed in samples with hydrocarbon-oxidising microorganisms, up to 89%. Algae also showed a significant reduction in oil concentration, about 72%, due to their ability to absorb and transform hydrocarbons. Vermiculture showed moderate efficiency, removing up to 65% of pollutants, confirming its potential as an additional clean-up method. No significant changes in oil content were found in the control group. These data indicate the possibility of a combined application of biological agents to improve bioremediation efficiency.

The results of the study confirm the promising use of microorganisms, algae and vermiculture in the processes of cleaning the marine environment from oil contamination. These methods can be adapted to different environmental conditions and integrated into existing water treatment systems. Future research should focus on the mechanisms of interaction between these biological agents and their combined application in natural ecosystems.

Keywords: Bioremediation, hydrocarbon-oxidising microorganisms, algae, vermiculture, oil pollution

References

1. Zhao, X., et al./ Polycyclic Aromatic Hydrocarbons Degradation by Algae-Microbe Consortia. Applied En□vironmental Microbiology, 2018, 84(11), e00345-18.
2. Juan C.Sanchez-Hernandez, C.Narvaez, X. Andrade Cares, P.Sabat, R.Naidu /Predicting the bioremediation potential of earthworms of different ecotypes through a multi-biomarker approach. Science of The Total Environment, 2023, V.862 https://doi.org/10.1016/j.scitotenv.2022.160547

Obtaining Dimethyl Ether in the Process of Biomimetic Oxidation of Methane with Hydrogen Peroxide

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Abstract

The production of dimethyl ether (DME) is gaining increasing attention as a promising, environmentally friendly and sustainable alternative to diesel fuel due to its high cetane number, low autoignition temperature and low pollutant emissions [1]. The addition of DME to liquefied petroleum gases reduces CO_2 emissions and reduces NOx emissions by 5–15% compared to [2] liquefied gases. The growing demand for methanol and DME requires the search for new methods of single-stage direct conversion of methane using effective catalysts within the framework of "green technologies" that allow methane to be oxidized with high selectivity at relatively low temperatures and pressures.

The methane monooxidation process was carried out in a flow-through quartz reactor with a special design, which provides the input of H_2O_2 into the reaction zone, with a volume of 3.5 cm3 in the ideal displacement mode at atmospheric pressure with varying process parameters - temperature t = 130-350 °C, volumetric feed rates of the initial reagents V_{CH_4}= 0.3-1.047 l/h, $V_{H_2O_2}$ = 1.47-5 ml/h, and the concentration of the oxidizer C_{H2O2} = 15-35%. The reaction products were analyzed using a 7820A GC System gas chromatograph from Agilent Technology and an LXM 80 chromatograph [3].

To obtain DME, a biomimetic catalyst was used, which showed high activity in the direct oxidation of methane with the green oxidizer H_2O_2. The biomimetic catalyst was synthesized on the basis of a modified fluorinated iron porphyrin complex, applying it to Al_2O_3 with a specific surface area of 236 m^2 /g An experimental study of the direct oxidation of methane to DME on a biomimetic catalyst was carried out depending on the process parameters, the results of which are presented in Figures 1 and 2. As can be seen from these figures, with an initial change in temperature and contact time, the DME yield increases to a maximum value of 8.2% at 250˚C and 10% at τ = 3.2 s, the conversion of CH_4 under these conditions was 24.3% and 24.8%, respectively [4,5].

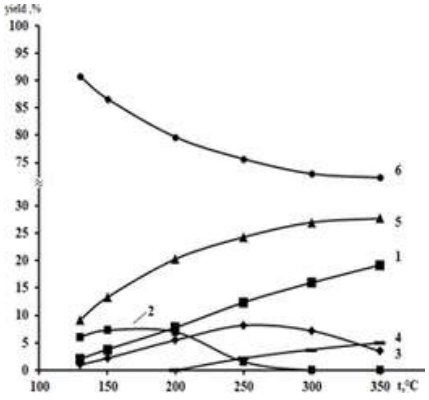

Fig 1.
Temperature dependence of reaction products of methane biomimetic oxidation by hydrogen peroxide

V_{CH_4}= 0,35 [l/h]; $V_{H_2O_2}$ =1,8[ml/h]; $C_{H_2O_2}$=30%; CH_4:H_2O_2=1:1; τ=2.45[sec.];

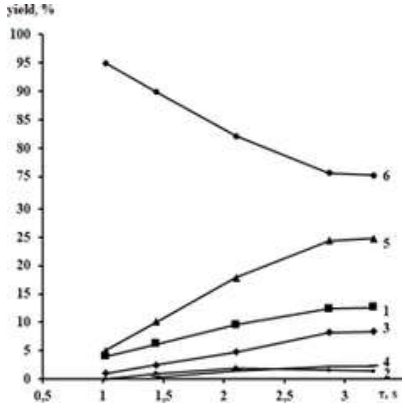

Fig 1.
Effect of contact time on the methane monooxidation reaction under the following conditions/Al_2O_3;$C_{cat.}$= 0.64 [mg/g]; t=300°C;

V_{CH_4}= 0.51 [l/h] $V_{H_2O_2}$ = 1.25[ml/h] ; $C_{H_2O_2}$=30%

1– CH_3OH; 2 – CH_2O; 3 – CH_3OCH_3; 4 – CO_2; 5 – CH_4 conversion; 6 – consumption of H_2O_2 in the catalase reaction

Conclusion

In the one-stage oxidation process of methane with hydrogen peroxide to penta-FTPhPFe3+/Al_2O_3, carried out in one reactor, along with methanol, a significant amount of dimethyl ether is obtained.

Keywords: Methane, Dimethyl ether, Biomimetic catalyst

References

1. Arcoumanis, C.; Bae, C.; Crookes, R.; Kinoshita, E. The potential of dimethyl ether (DME) as an alternative fuel for compression-ignition engines: A review. Fuel (2008) 87, pp.1014– 1030.
2. Han, S.; Sik, C. Applicability of dimethyl ether (DME) in a compression ignition engine as an alternative fuel. Energy Convers. Manag. (2014) 86, pp.848–863. 126 Materials and Technologies for Advanced Engineering Research
3. Patent AZ, № İ 20220060, T.M. Nagiev, L.M. Gasanova, G.Ch. Nahmatova., "Method of methanol obtaining", 27.09.2022.
4. Gulshan Nahmatova, Latifa Gasanova, Olga Vodyankina, Eldar Dakhnavi, Tofik Nagiev, Coherently synchronized reaction of methane oxidation by green oxidizing agent – hydrogen peroxide over the biomimetic catalyst – iron pentafluorotetraphenylporphyrin deposited on alumina, Reaction Kinetics, Mechanisms and Catalysis, (2022) V.135, pp.3285-3301. https: doi.org/10.1007/s11144-022-02300-z
5. Gulshan Nahmatova, Latifa Gasanova, Tofik Nagiev “Study of the Methanol Conversion into Dimethyl Ether Obtained in the Process of Biomimetic Methane Monooxidation by Hydrogen Peroxide “ Materials Science Forum Submitted: Vol. 1121, pp 119-128 ,14.05.2024

Phase Equilibria and Magnetic Properties of $Mn_xGe_{2-x}Sb_2Te_5$ Solid Solutions

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Abstract

Magnetic topological insulator candidates $Mn_2Bi_2Te_5$ and its sister compound, $Mn_2Sb_2Te_5$, have the same tetradymite-like layered crystal structures. These materials consisting of $(A^{IV}Te)_2$ bilayers intercalated between $Bi(Sb)_2Te_3$ quintuple layers crystallize in a hexagonal structure with $P\bar{3}m1$ (No. 164) space group. Their layered structures consist of repeating units known as nonuple layers, which stack along crystallographic c axis and are separated by van der Waals gaps. There exist only two published studies on $Mn_2Sb_2Te_5$, one of which [1] shows that depending on how nonuple layers and $(MnTe)_2$ sublattices stack, it may be either an antiferromagnetic topological insulator or a Dirac semimetal. The study also predicts that although $Mn_2Sb_2Te_5$ with ideal and defects-free lattice has an AFM ordering irrespective of stacking, deviation from stoichiometry and site mixing between Mn and Sb atoms in experimental samples can result in ferrimagnetic ordering. The existence of very few studies coupled with only one study on experimental realization of $Mn_2Sb_2Te_5$ [2] seems to highlight more of a difficulty in obtaining it rather than an interest in studying it experimentally. An analogous compound, $Ge_2Sb_2Te_5$, is a well-known phase-change material [3], which is predicted to possess a nontrivial band topology if site mixing between Ge and Sb atoms is taken into account [4]. Due to the close similarity in the ionic sizes of Mn^{2+} and Ge^{2+}, substitution of Mn at Ge site in $Ge_2Sb_2Te_5$ can be attempted to identify possible formation of homogeneous solid solutions. Though a solubility limit may put a limit on magnetism, a higher chemical stability coupled with nontrivial band topology can be achieved.

Here, we present polycrystalline $Mn_xGe_{2-x}Sb_2Te_5$ solid solutions synthesized via a high-temperature solid-state reaction and study of their structural and magnetic properties to assess feasibility of formation of homogeneous solid solutions and existence of magnetic transitions. Powder X-ray diffraction and differential thermal analysis showed that Ge atoms were successfully substituted by Mn atoms in the composition range from x=0 to x=1 as the solid solutions possessed single-phase purity and homogeneity in this range. Rietveld refinement revealed that substitution of Mn led to changes in the arrangement of atoms in the crystal structure with an overall lattice contraction due to the smaller radii of the Mn atoms. In addition, magnetic measurements showed that substituting Ge atoms with Mn atoms led to emergence of ferrimagnetic ordering at low temperatures with a distinct magnetic transition temperature, which leads to a paramagnetic ordering upon heating. Both magnetic transition temperature and net magnetization linearly increases in proportion to substitution of Mn with a distinct magnetic transition temperature starting to appear at x=0.6. Therefore, as magnetic ordering besides single-phase purity and homogeneity exists in this range, growth of single crystals can be attempted in the composition range of x=0.6 to x=1 with priority given to Mn-rich compositions. The grown single crystals, which hold promise for future as magnetic topological insulators, can then be investigated in terms of magneto-transport properties, topological states, and van der Waals heterostructures involving their coupling with other magnetic or nonmagnetic topological insulators.

Keywords: Methane, Dimethyl ether, Biomimetic catalyst.

References

1. S.V. Eremeev, M.M. Otrokov, A. Ernst, E.V. Chulkov, Magnetic ordering and topology in $Mn_2Bi_2Te_5$ and $Mn_2Sb_2Te_5$ van der Waals materials, Phys. Rev. B 105 (2022) 195105. https://doi.org/10.1103/PhysRevB.105.195105.
2. A. Saxena, V.P.S. Awana, Growth and characterization of the magnetic topological insulator candidate $Mn_2Sb_2Te_5$, J. Phys. Condens. Matter 36 (2023) 085704. https://doi.org/10.1088/1361-648X/ad0c77.
3. B.J. Kooi, J.Th.M. De Hosson, Electron diffraction and high-resolution transmission electron microscopy of the high temperature crystal structures of $Ge_xSb_2Te_{3+x}$ (x=1,2,3) phase change material, J. Appl. Phys. 92 (2002) 3584–3590. https://doi.org/10.1063/1.1502915.
4. S.V. Eremeev, I.P. Rusinov, P.M. Echenique, E.V. Chulkov, Temperature-driven topological quantum phase transitions in a phase-change material $Ge_2Sb_2Te_5$, Sci. Rep. 6 (2016) 38799. https://doi.org/10.1038/srep38799.

The Investigation of K+ Salts of Amidoamines Synthesized in Various Mole Ratios of Ethylenediaminetetraacetic Acid with Diethanolamine as Corrosion and Salt Precipitation Inhibitors

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Abstract

The presented work is devoted to the synthesis of K+ salts of amidoamines based on EDTA and diethanolamine (DEA), and their study as corrosion and salt deposition inhibitors. To do this work, we first obtained complexes of EDTST with DEA in different molar ratios (1:1-1:3) at room temperature, then we converted these complex compounds into amidoamines by heating them at 120-150^{0}C for 2 hours, and their salts were obtained by treating these amidoamines with 20% KOH.

The structures of the synthesized salts were confirmed by recording the IR spectra in the 400- 4000 cm^{-1} wavenumber range on the “Alpha” IR Fourier spectrometer of the German company BRUKER. Their 10% solutions were prepared, their physicochemical parameters were determined, and studies were carried out as corrosion and salt precipitation inhibitors.

Metals corrode and fail as a result of chemical and electrochemical reactions. Along with losses due to corrosion, serious fires and explosions often occur. Damage to nature due to the spillage of toxic chemicals and oil products into the environment as a result of accidents caused by corrosion is immeasurable. Intensive pollution of the atmosphere, water and soil as a result of the rapid development of technology makes the environment more aggressive towards metals and their alloys. Corrosion occurs in all areas of industry, as well as in agriculture, and creates major problems [1-3]. Corrosion of military equipment is more dangerous. In order to prevent corrosion, there is a great need for the synthesis of environmentally friendly and effective inhibitors [4]. Na+, K+ salts of amidoamines synthesized on the basis of ethylenediaminetetraacetic acid (EDTA) and alkylamines have both anti-corrosion and bactericidal effects in the aquatic environment.

The presented work is devoted to the synthesis of K+ salts of amidoamines based on EDTA and diethanolamine (DEA), and their study as corrosion and salt deposition inhibitors. To do this work, we first obtained complexes of EDTA with DEA in different molar ratios (1:1-1:3) at room temperature, then we converted these complex compounds into amidoamines by heating them at 120-150^{0}C for 2 hours, and their salts were obtained by treating these amidoamines with 20% KOH.

The structures of the synthesized salts were confirmed by recording the IR spectra in the 400- 4000 cm^{-1} wavenumber range on the “Alpha” IR Fourier spectrometer of the German company BRUKER. Their 10% solutions were prepared, their physicochemical parameters were determined.

Metal plates were placed in these solutions, and studies as corrosion and salt deposition inhibitors were conducted in concentrations of 50, 100, 150 mg/l for 5 hours using a known methodology. The results obtained are given in Table.

Table. Investigation of 10% solutions of K+ salts of synthesized amides in different molar ratios of EDTST with DEA as corrosion and salt precipitation inhibitor

The name of the substance	The density of the substance C, mg/l	Corrosion rate P, /m²h		Protective effect, Z	
		Inhibitor-free	with an inhibitor	From corrosion	From salt precipitation
1	2	3	4	5	6
Amidine K salt synthesized from EDTA with DEA in a 1:1 molar ratio	50 100 150	0,4 0,4 0,4	0,1 0,09 0,7	56 65 72	52 63 69
Amidine K salt synthesized from EDTA with DEA in a 1: molar ratio	50 100 150	0,5 0,5 0,5	0,2 0,17 0,14	55 61 70	50 59 68
Amidi ne K salt synthesized from EDTA with DEA in a 1:3 molar ratio	50 100 150	0,7 0,7 0,7	0,1 0,09 0,08	53 59 67	51 58 65

It can be seen from the table that the 10% solution of the K+ salt of the synthesized amide of EDTA with DEA in a 1:1 molar ratio protects metal plates from corrosion by 56% at a concentration of 50 mg/l, and salt precipitation is 52%. At concentrations of 100 and 150 mg/l, metal plates are protected from corrosion by 65 and 72%, and salt deposition is 63 and 69%.

A 10% solution of the K+ salt of amidine synthesized in a 1:2 molar ratio protects metal plates from corrosion by 55% at a concentration of 50 mg/l, and the salt deposition is 50%. At concentrations of 100 and 150 mg/l, the metal plates are protected from corrosion by 61 and 70%, and the salt deposition is 59 and 68%.

A 10% solution of the K+ salt of amidine synthesized in a 1:3 molar ratio protects metal plates from corrosion by 53% at a concentration of 50 mg/l, and the salt deposition is 51%. At concentrations of 100 and 150 mg/l, the metal plates are protected from corrosion by 59 and 67%, and the salt deposition is 58 and 65%.

Keywords: ethylendiaminetetraacetic acid, diethanolamine, salt precipitation.

References

1.Koch G.H., Brongers P.H., Thompson N.G., Virmani V.P., Payer J.H//Wachington D.C. HWA, 2002-URL http//rosap.ntl.bts.gov/view/dot/40697

2. Koch G.H., Thompson N.G., Moghiss O., Payer J.H., Varnes, Impact NACE. International Measures of Prevention application and economics of corrosion technologies, Houston NACE International, 2016- URL http//:www.nae.edu/155346/NACE-Internationals-IMPACT-Study-Breaks-New-Ground in-Corrosion-Management-Research-and-Practise

3. Kats N.G., Starikov V.P., Parfenova S.N. Chemical resistance of materials and protection of oil and gas processing equipment: a tutorial, M. Mashinostroenie, 2011, -436 p. 4. Abbasov V.M., “Corrosion”, Baku-2007, 348 p.

Synthesis, Characterization, Crystal Structure, and Physiological Studies of Cu(II) Complexes with Nitrogen-containing Ligand

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Abstract

Two new mononuclear Cu(II) complexes with the nitrogen-containing ligand N2-(4- methylpyridin-2-yl)-N6-(pyrazin-2-yl)-pyrazine-2,6-diamine (H_2pcpzpzda) were synthesized and their crystal structures were analyzed in detail by X-ray diffraction. In both Cu(II) complexes, (H_2pcpzpzda) acts as a tridentate ligand and has an octahedral geometry with the metal atom. The binding of the amine groups to the Cu(II) metal in both complexes resulted in the calculation of their physiological performances with acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibitors. The IC50 values for the Cu(II) complexes against the AChE inhibitor were 6.70 μM and 1.42 μM, respectively, indicating dual inhibitory efficacy. Also, in vitro calculations revealed that the complexes also exhibited dual inhibitory efficacy against BChE-inhibitor, with IC50 values of 45.70 μM and 27.72 μM, respectively. In addition, molecular docking and molecular dynamics were studied for both complexes and enzymes.

Two Cu(II) complexes were synthesized by the reaction of H_2pcpzpzda and the corresponding Cu(II) salts in methanol. The Cu(II)-1 complex was synthesized by the direct reaction of H_2dpzpda and $Cu(NO_3)_2{\cdot}3H2O$ and $Cu(CH_3COO)_2H_2O$ salts in methanol. Single crystals obtained by slow diffusion of ethyl ether into methanol solution were used for X-ray diffraction analysis [1-5]. Mononuclear Cu(II) complexes were prepared by the treatment of $Cu(NO_3)_2{\cdot}3H_2O$ and $Cu(CH_3COO)_2H_2O$ with the ligand H_2dpzpda in methanol. Single crystals obtained by diffusion of ethyl ether into methanol solution were used for X-ray single crystal analysis. In both complexes, the metal atom was linked to 3 nitrogen atoms. Alzheimer's disease is the most common neurological disease in society, but when it comes to treating Alzheimer's disease, there are not many drug options. The most important of these drugs are cholinesterase inhibitors. Cholinesterase inhibitors correct the reduced levels of acetylcholine that cause memory loss and cognitive dysfunction in these patients. The structures of both AChE and BChE inhibitors have been elucidated, and potent compounds are now being created through Our goal in synthesizing these complexes is to synthesize chemical compounds that will help create more effective drugs.rational designs.

Keywords: Cu(II) complexes, crystal strucrture, physiological studies.

References

1. Author, F.: Article title. Journal 2(5), 99–110 (2016).
2. Homepage, http://www.website.com/ , last accessed year/month/day.
3. Sheldrick, G.M. Acta Cryst, A64, 1122008.
4. Sheldrick, G. M. Acta Cryst. 2015, C71, 3.
5. APEX3, Bruker AXS Inc. Madison Wisconsin USA (2013).

Pyrolysis and Briquetting of Biomass: An Effective Approach to Sustainable Energy Production

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Abstract

In recent years, global challenges such as environmental protection and ensuring energy security have significantly increased interest in renewable energy sources. Within this context, the production of biofuels from biomass has emerged as a sustainable alternative from both ecological and economic perspectives. Technologies such as biomass pyrolysis and briquette production not only enable efficient waste management but also play a crucial role in diversifying energy systems.

This study provides an in-depth analysis of the role of these technologies in the biofuel sector, evaluating their environmental advantages and potential applications from various angles. Research indicates that biomass pyrolysis and briquetting hold strategic importance in biofuel production. These processes contribute to the generation of renewable energy and effective waste management, while also helping to reduce greenhouse gas emissions and lessen dependence on limited energy resources[1-4].

Biomass pyrolysis is considered one of the most promising methods for biofuel production, particularly due to its potential for bio-oil generation. Studies focused on thermochemical processes and catalysts have made it possible to obtain high-quality biofuels with minimal environmental impact, making them suitable for use in transportation and heating systems[3,5].

On the other hand, briquettes made from biomass are used as solid biofuels to meet various energy needs. Research into their energy density, combustion characteristics, and emission profiles has shown that they present a cleaner and more sustainable alternative to traditional solid fuels [1,2].

Moreover, integrating biomass pyrolysis with briquette production offers a comprehensive and efficient approach. This integration ensures more effective utilization of raw materials and contributes to the advancement of bioenergy systems and the transition to a low-carbon economy[5,6].

Analysis of pyrolysis processes and energy values As part of the study, pyrolysis of pine wood sawdust was carried out at temperatures ranging between 400–500°C. Based on the raw material's composition—carbon (52.50%), hydrogen (5.80%), and oxygen (40.10%)—its calorific value was calculated using the Dulong formula, resulting in approximately 18.88 MJ/kg. Other analytical indicators are presented in the table below.

Proximate, Compositional, and Elemental Analysis of Biomass Sample

Analysis Type	Parameter	Adjusted Value (%)
Proximate Analysis	Moisture	9.40
	Volatile Matter	81.00
	Fixed Carbon	9.00
	Ash	0.35
Compositional Analysis	Extractives	6.30
	Holocellulose	71.00
	Hemicellulose	22.90
	Cellulose (by difference)	48.30
	Lignin	26.30
	Oil/Fat	3.30
Ultimate Analysis	Carbon	52.50
(dry, ash-free basis)	Hydrogen	5.80
	Nitrogen	1.60
	Oxygen (by difference)	40.10
Molar Formula	Empirical Formula	$CH_{1.34}N_{0.02}O_{0.57}$
Atomic Ratios	H/C	1.34
	O/C	0.57
Energy Content	Higher Heating Value (HHV)	19.10 MJ/kg

Research has shown that biomass pyrolysis and briquetting hold great potential as environmentally friendly, energy-efficient, and sustainable alternatives. These technologies not only contribute to effective waste management but also support the expansion of renewable energy sources.

By converting agricultural and forestry residues into valuable fuel, these processes help reduce the environmental burden of waste while offering a reliable and cleaner source of energy. Moreover, they align with global efforts to transition to low-carbon energy systems, making them particularly relevant in the fight against climate change. As innovation continues in the field of bioenergy, the integration of pyrolysis and briquetting technologies is expected to play an increasingly important role in shaping a more sustainable energy future.

Keywords: Biomass, fuel, briquettes, wood, alternative energy pyrolysis

References

1. Hasankhanova N., Salahova F. «Investigationof thermal and thermocatalytic convertion process of vacuum gas oil and its mixture with vegetable oil.» Procedings of Azerbaijan high technical educational institutions.Vol.39(05) ISSUE 04 2024pp.425-432.
2. Hasankhanova N.V., Nasirov F.A. "Production and research of fuel briquettes based on epoxidized vegetable oils and waste of cultivated plants" // 19th Asian Chemical Congress, 2023. Vol.45(02), ISSUE 03, pp.123-135.
3. http://www.ecoproject.org/projects/biomass_brochure.pdf
4. http://www.kimyamuhendisi.com/dokumanlar/15-enerji-sistemleri.html, ET: 12.2009.
5. Oliveira, P. E., Leal, P. & Pichara, C. E. Pellets derived from Eucalyptus nitens residue: physical, chemical, and thermal characterization for a clean combustion product made in Chile. Can. J. For. Res. 48, 1194–1203. https://doi.org/10.1139/cjfr-2018-0122 (2018)
6. Вавилов А.В. Брикеты из возобновляемых биоэнергоисточников. Монография. /А.В. Вавилов// Минск, Стринко, 2013

Investigation of Phase Equilibria and Topological Insulator Phases in the SnTe-PbTe-Bi_2Te_3 ternary system

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Abstract

The A^{IV}–B^{V}–Te systems (where A^{IV} can be Ge, Sn, Pb and B^{V} can be Sb, Bi) with the formula $A^{IV}_{m}B^{V}_{2n}Te_{3n+m}$ are indeed three-dimensional topological insulators, characterized by their insulating bulk and gapless surface states, and exhibit unique quantum properties suitable for advanced technological applications [1, 2]. These materials exhibit a complex multilayered structure, composed of covalently bonded blocks stacked along the c-axis, with each block connected by weak van der Waals interactions. Notably, intermediate compositions display interesting electrical behaviors, including a potential enhancement of the thermoelectric power factor ($S^2\sigma$) [3]. The presented work shows the results of the study of solid-state equilibria in the SnTe-PbTe-Bi_2Te_3 system.

Alloys of the studied system were prepared on different cross-sections in order to construct the whole phase diagram. Each sample was prepared with a total weight of 0.5 grams. All alloy samples were first placed in a furnace at 1000 K for 5 h and then water quenched. Subsequently, they were annealed at 700 K for 1000 h to form equilibrium phases.

The melting temperatures of the synthesized alloys were determined using differential thermal analysis (DTA) with a LINSEIS HDSC PT1600 system (accuracy ±2 K), applying a heating rate of 10 K/min. Phase compositions were analyzed by X-ray diffraction (XRD) using a Bruker D2 PHASER diffractometer with CuKα_1 radiation, within a scanning range of 2θ = 5–75°. Microstructural analysis was carried out using a Tescan Vega 3 SBH scanning electron microscope (SEM) equipped with a Thermo Scientific UltraDry Compact EDS detector.

An isothermal section at 300 K for the SnTe–PbTe–Bi_2Te_3 system was constructed based on XRD and SEM analyses of equilibrated alloys, as illustrated in the Figure. As shown in Figure, there are seven single-phase exists in the SnTe–PbTe–Bi_2Te_3 system: β-phase based on Bi_2Te_3, α-phase based on PbTe, continuous solid solution fields formed on the sections $SnBi_2Te_4$–$PbBi_2Te_4$, $SnBi_4Te_7$–$PbBi_4Te_7$, $SnBi_6Te_{10}$–$PbBi_6Te_{10}$, respectively, γ-, δ-, ε-phases, and η- and φ-phases based on $Sn_2Bi_2Te_5$, $Sn_3Bi_2Te_6$ compounds. These solid solution fields lead to the formation of several two- and threephase fields in the system

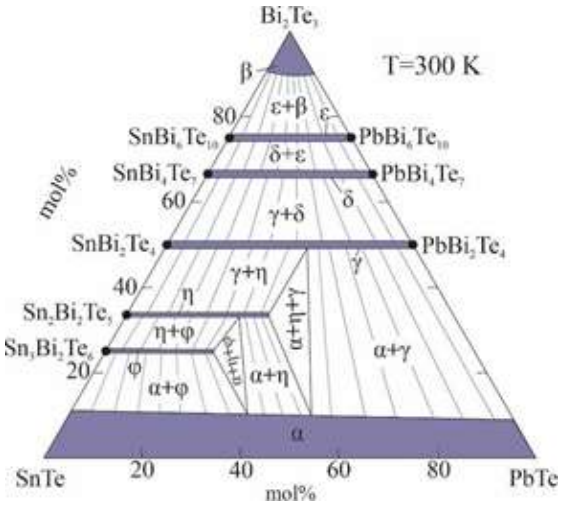

Figure. Isothermal sections of the SnTe-PbTe-Bi_2Te_3 system

In this study, the phase equilibria within the SnTe-PbTe–Bi_2Te_3 compositional area of the Pb–Sn–Bi–Te system were experimentally investigated for the first time. The formation of a wide range of solid solutions based on ternary compounds has been observed. The newly synthesized and characterized phases are of significant interest due to their potential applications as bismuth-based topological insulators and thermoelectric materials.

Keywords: layered bismuth tellurides, solid solutions, phase diagram, tetradymite-like structure, topological insulator

References

1. Shen, S.Q. Three-Dimensional Topological Insulators. In: Topological Insulators. Springer Series in Solid-State Sciences, 187. 280 p (2017).
2. Babanly, M.B., Chulkov, E.V., Aliev, Z.S., Shevelkov, A.V., Amiraslanov, I.R. Phase Diagrams in Materials Science of Topological Insula-tors Based on Metal Chalcogenides. Russian Journal of Inorganic Chemistry. 62. 1703–1729 (2017).
3. Kuropatwa, B.A, Kleinke, H. Thermoelectric Properties of Stoichiometric Compounds in the (SnTe)x(Bi2Te3)y System. Zeitschrift für anorganische und allgemeine Chemie. 638(15). 2640-2647 (2012)

Investigation of the UV-Vis Analysis Results of Silver Nanoparticles Synthesized in a Gelatin Matrix

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Abstract

Over the past decade, silver nanoparticles (AgNPs) have been increasingly incorporated into a wide variety of consumer products [1]. Their chemical synthesis typically involves the use of reducing agents in the presence of stabilizers to prevent undesirable agglomeration. In aqueous environments, AgNPs are inherently unstable and prone to aggregation due to their high surface reactivity. However, this tendency can be significantly mitigated through the use of suitable stabilizing agents. A broad spectrum of polymers has been explored for this purpose, demonstrating effective stabilization of AgNPs in solution [2].

In this study, polymer/Ag-based complexes were synthesized for this purpose. Natural polymer gelatin was used as the stabilizing agent. A silver solution amounting to 10% of the polymer mass was added to the polymer [3]. The properties of the resulting composite were investigated using physico-chemical analysis methods. Based on UV-Vis analysis, the size of the silver nanoparticles was determined.

UV-Vis spectroscopy is a widely used analytical technique for monitoring the formation of complexes between inhibiting compound molecules and metal ions within an electrolyte solution. Based on the UV analysis results, a comparison was made between gelatin, gelatin/Ag, and gelatin/Ag/Reducing agent solutions. In the gelatin solution, maximum absorption was observed at 340 nm, which corresponds to the ultraviolet light absorbed primarily by the amino acids and peptide bonds present in gelatin. Upon complexation of Ag+ ions with gelatin, an increase in absorbance was observed, with a new absorption maximum at 450 nm. After the addition of a reducing agent to the solution, the maximum absorption wavelength (λmax) was determined to be 399.20 nm.

Thus, the obtained results indicate that silver nanoparticles were stabilized within the gelatin matrix. The appearance of the peak around ~400 nm suggests the formation of small nanoparticles (~10 nm), approximately in size. These data are consistent with the literature; a previous study reported a plasmon resonance peak near 400 nm for silver nanoparticles with a size of 12 ± 2 nm [4].

Keywords: gelatin, silver nanoparticles, UV-vis spectroscopy

References

1. Abo-Elmagd, R.A., Hamouda, R.A. & Hussein, M.H. Phycotoxicity and catalytic reduction activity of green synthesized Oscillatoria gelatin-capped silver nanoparticles. Sci Rep 12, 20378 (2022). https://doi.org/10.1038/s41598-022-22976-6
2. Lim Jeong and Won Ho Park//Preparation and Characterization of Gelatin Nanofibers Containing Silver Nanoparticles// International Journal of Molecular Sciences 2014, vol.15, p.6857-6879; doi:10.3390/ijms15046857
3. E.Babayev, N.Rahımlı, U.Mammadova, D.Babayeva//Synthesıs of polymer-based sılver nanopartıcles, structure and properties of obtaınedpolymer composite//INTERNATIONAL CERAMICS AND COMPOSITE MATERIALS SYMPOSIUM November 15-16, 2024, Süleyman Demirel University, Isparta, Türkiye, p.192-194.
4. S.F.Humbatova, N.A.Zeynalov, D.B.TAghıyev, S.Z.Tapdıqov, S.M.Mammedova//Chıtosan polymer composite materıal contaınıng of sılver nanopartıcle//Digest Journal of Nanomaterials and Biostructures Vol. 11, No. 1, January - March 2016, p. 39 – 44.

Meta-Benchmarking Study of Docking Protocols

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Abstract

Despite the wide-spread use of docking as a virtual screening tool, its performance is often disappointing – a well-known truth acknowledged by all practitioners of docking, and yet not visible from literature – which is significantly biased towards selectively publishing success stories only. In this contribution, we wish to provide the reader with a detailed, pedagogical insight of the problems affecting the calibration and benchmarking procedures of docking algorithms. We have critically evaluated current benchmarking and calibration methods according to the selection of the dataset, success criterion assessed by the authors the conclusions drawn by them. To support our hypothesis, we used our in-house docking tool S4MPLE for an in-depth exploration of its behaviour and performances with respect to the tuneable parameters of its energy function. Our findings indicate that despite docking being a fundamental methodology in drug design, it is still possible to see common mistakes in literature, including inconsistent terminology usage, artificially generated dataset usage for calibration and benchmarking, inadequate metrics for post-mortem analysis, and poorly defined success criteria for parameter optimization protocols. Furthermore, our results of docking calculation from S4MPLE over 7 targets and more than 300 ligands, which likely apply to any other docking protocol, suggest that it is relatively easy to calibrate a docking "score" to achieve state-of-the-art native pose prediction results in redocking. Many different setups are seen to lead to near-optimal results in this respect: however, each of these setups may return radically different rankings of poses and ligands in terms of energy/affinity/score. Therefore, we suggest that docking calibration and benchmarking should always include, in a multi objective optimisation approach, both pose prediction and active compound retrieval criteria – the latter using as far as possible real activity data rather than artificial active/decoy sets.

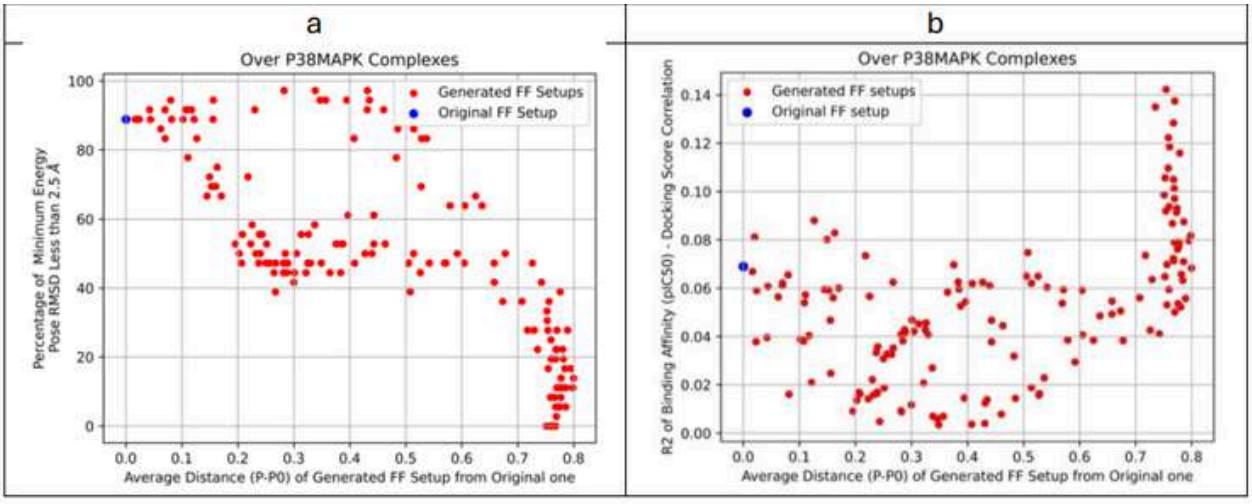

Figure 1. Performances of generated FF setups on pose ranking (a) and virtual screening (b) over P38MAPK complexes as an example

Keywords: Protein-Ligand Docking, Benchmarking, Calibration.

References

1. Laurent Hoffer; Dragos Horvath. S4MPLE--sampler for multiple protein-ligand entities: simultaneous docking of several entities. J Chem Inf Model. 2013, 28;53(1), 88-102.

2. Tran-Nguyen, V.-K.; Rognan, D. Benchmarking Data Sets from PubChem BioAssay Data: Current Scenario and Room for Improvement. IJMS 2020, 21 (12), 4380

The Study of Composites Based on Modified Tripolymer Ethylene-Propylene Rubber

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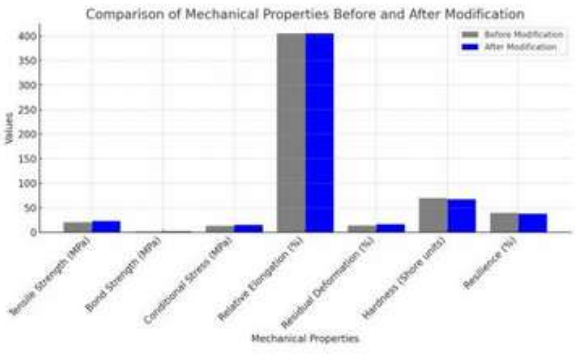
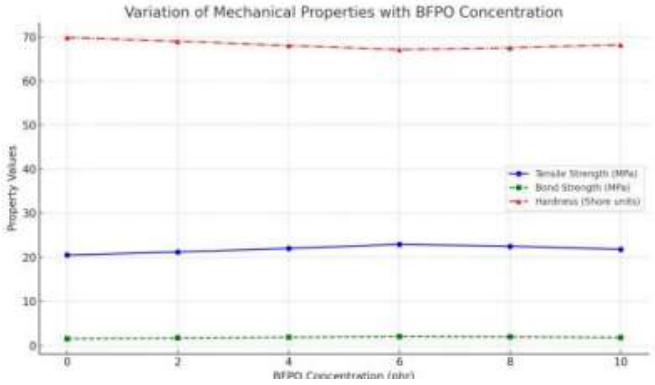
Abstract

The modification of ternary ethylene-propylene rubber (SKEPT-60) plays a crucial role in enhancing its mechanical properties and industrial applications. This study explores the impact of benzaminated phenol-formaldehyde oligomer (BFPO) as a modifying agent to improve compatibility with other materials, particularly butadiene-nitrile rubber. The research aims to enhance the rubber's tensile strength, bond strength, and other key properties, making it more effective for various industrial uses. Previous studies have focused on different modification techniques, but limited research exists on BFPO's specific effects on SKEPT-60.

The study involves the preparation of binary mixtures of SKEPT-60 and BFPO under controlled laboratory conditions. The mixture is synthesized at temperatures between 40-60°C for 25 minutes, followed by vulcanization at 153±20°C for 30 minutes. The rheological properties of the modified rubber are analyzed to determine the optimal BFPO content for maximizing material performance. Mechanical testing is conducted to assess tensile strength, bond strength with metal, hardness, resilience, and other key physical properties. The impact of different BFPO concentrations is systematically evaluated.





Experimental findings demonstrate that BFPO modification significantly improves key mechanical properties of SKEPT-60. The tensile strength increases by 12%, while bond strength with metal surfaces improves by up to 30%. The composition exhibits tensile strength values ranging between 20.5 and 22.9 MPa, with conditional stress at 300% elongation varying from 13.0 to 14.9 MPa. The relative elongation reaches 405%, whereas residual deformation increases from 13.8% to 16.0%. A slight reduction in hardness is observed, decreasing from 69.8 to 67.1 Shore units. Bond strength with metal ranges from 1.52 to 2.01 MPa, and resilience upon rebound decreases slightly from 39.6% to 37.8%. The optimal BFPO content of 4-6 phr results in a 10-12% improvement in primary characteristics.

The study confirms that modifying ternary ethylene-propylene rubber with BFPO enhances its mechanical performance and adhesion properties, making it more suitable for industrial applications. The improvements in tensile strength, elongation, and bond strength indicate that this modification method can contribute to the development of more durable and efficient composite materials. These findings provide valuable insights for industries utilizing modified rubber in manufacturing and engineering applications.

Keywords: Ethylene-propylene rubber, benzaminated phenol-formaldehyde oligomer, modification, mechanical properties, compatibility, industrial applications

References

1. Investigation of the rheological structural parameters of a network of NBR-based vulcanizates with theparticipation of chlorine-containing, Journal of new technology and Materials, Vol 13, ISSUE 1,2

2. .Amirli F.A., Movlayev İ.H. Compositions based on modified epoxy oligomer. Processes of Petrochemistry and Oil Refining, PPOR, №3, 2024, pp.786-792 https://doi.org/10.62972/1726-4685.2024.3.786

3. Amirli F.A., Movlayev I.H., Mammadova A.F. Study of the rheology properties of the mixture of terminal ethylene-propylene rubber with benzynamine-modified phenol-formaldehyde oligomer. PPOR,Vol. 26, No. 1, 2025, pp.229-239 https://doi.org/10.62972/1726-4685.2025.1.229

Computational and Statistical Approaches to Small Ring Conformational Analysis

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Abstract

Macromolecular crystallography and cryo-EM, despite being the primary techniques for 3D structure determination, produce noisy data. To mitigate this, Bayesian statistics is used, integrating data likelihood with prior knowledge. While the use of stereochemical information like bond lengths and angles is well-established, conformational angle analysis remains difficult, particularly for rings due to their inherent constraints. This research develops a framework for deriving, organising, and incorporating prior knowledge about small ring conformations by combining experimental data from the Crystallography Open Database (COD) with computational simulations from RDKit and PySCF.

A high-resolution (≤ 1.0 Å) dataset of X-ray crystal structures, containing discrete molecular entities, was curated from the Crystallography Open Database[1,2] (COD). All molecular structures within these entries were extracted, and non-aromatic rings, specifically those of four, five, and six members composed of carbon, nitrogen, oxygen, phosphorus, sulphur, or boron atoms, were identified. Ring classification was achieved through analysis of local atomic graph properties and atomic sequence. Subsequently, Cremer-Pople[3] parameters were calculated for each identified ring. To facilitate subsequent computational analysis, these ring classes were translated into SMILES strings. Conformational ensembles were generated utilising RDKit[4] , and conformational energies were calculated employing Density Functional Theory (DFT) and Hartree-Fock (HF) methods, implemented within the PySCF[5] software package.

From a set of 523,000 crystal structures within the COD, 235,000 were selected, meeting criteria for finite molecular entities and structural quality suitable for subsequent analysis. These structures yielded 450,000 molecules, among which 157,000 contained non-aromatic rings. A subset of 116,000 rings, composed of carbon, oxygen, nitrogen, phosphorus, sulphur, or boron, and ranging in size from three to six atoms, was identified. These rings were classified into 7,600 distinct ring classes, with only 20 classes exhibiting a sample exceeding 500 members. Recognising the thermodynamic dependence of conformational populations on energy differences (e.g., Boltzmann distribution), we proceeded to calculate the energies of all accessible conformations for each ring class. RDKit was employed for conformer generation, utilising SMILES string representations of the ring classes. Resulting conformers were superimposed, and only geometrically distinct conformers were retained for further analysis. Hartree-Fock and Density Functional Theory (DFT) methods were employed for energy calculations. The calculated energies were subsequently used to determine conformational probabilities and relative population sizes. This work is currently ongoing.

Preliminary analysis of COD data revealed that experimental observations alone are insufficient to sample the conformational space of all ring classes. Consequently, the incorporation of simulated data is essential. Although this work remains ongoing, initial results demonstrate the potential of combining experimental and simulated data for statistical modelling, thereby establishing prior knowledge applicable to structural biology analyses. The result of this work will improve the quality of structures in the PDB.

Keywords: Computational Structural Biology, Cheminformatics, Statistical Modeling

References

1. COD Database, https://www.crystallography.net/cod/, last accessed 2025/03/18.
2. Long, F., Nicholls, R. A., Emsley, P., Gražulis, S., Merkys, A., Vaitkus, A. & Murshudov, G. N. (2017). AceDRG: a stereochemical description generator for ligands. Acta Cryst. D73, 112â 122.
3. Cremer, D., Pople, J.A.: A General Definition of Ring Puckering Coordinates. J. Am. Chem. Soc. 97(6), 1354–1358 (1975).
4. RDKit: Open-Source Cheminformatics Software : https://www.rdkit.org/ last accessed 2025/03/18.
5. Quantum chemistry with Python : https://pyscf.org/ last accessed 2025/03/18.

Copper(II) monohelix Complex with Pyrimidine-modulated Long-chain Oligo-α-aminopyridine Ligand: Synthesis and Crystal Structure

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Abstract

The oligo-α-pyridyl/pyrimidinyl/pyrazilamine ligands, which have numerous pyridine, pyrimidine, pyrazine, and amino groups, have attracted increasing attention over the past three decades because of their capability to form "Extended Metal Atom Chain Complexes" (EMACs), which have a potential for molecular metal wires and switch applications [1,2]. Here we report for the first time the syntheses of N^2-(pyridin-2-yl)- N^6-(6-((6-((6-(pyrimidin-2-ylamino)pyridin-2-yl)amino)pyridin-2-yl)amino)pyridin-2-yl)pyridine-2,6-diamine (H_5N_{11}-tpm) (1) ligand and its corresponding mononuclear copper(II) complex—$[Cu(H_5N_{11}\text{-tpm})](ClO_4)_2$(2). The ligand H_5N_{11}-tpm was synthesized by the palladium-catalysed cross-coupling of 2-aminopyridine and N^2 - (6-bromopyridin-2-yl)-N^6-(6-((6-(pyridin-2-ylamino)pyridin-2-yl)amino) pyridin-2-yl)pyridine-2,6-diamine in the presence of catalysts [$Pd_2(dba)_3$, BINAP, ButONa] in refluxing toluene under argon and characterized by elemental analyses, IR, 1H NMR, and MS (FAB). (2) was synthesized by reacting copper(II) perchlorate with the H_5N_{11}-tpm ligand in methanol and characterized by X-ray crystallography. The crystal structure of 2 is shown in Fig. 1.

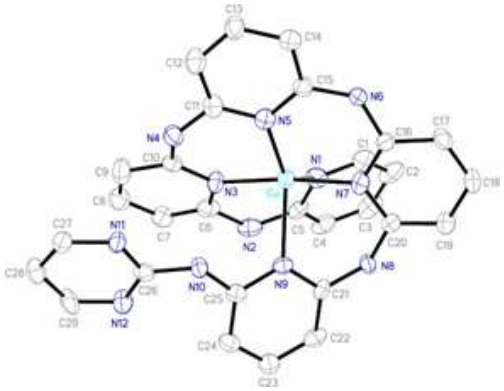

Fig.1. The molecular structure of the $[Cu(H_5N_{11}\text{-tpm})]^{2+}$ in 2. Thermal ellipsoids are drawn at the 50% probability level.

Complex 2, $C_{29}H_{24}Cl_2CuN_{12}O_8$, crystallizes in the orthorhombic system with space group Pbcn. In complex 2, Cu(II) is five-coordinated in an N_5 environment formed by nitrogen atoms of five pyridine rings of H_5N_{12}-tpm ligand (Fig.1). In complex cation $[Cu(H_5N_{11}\text{-tpm})]^{2+}$ copper(II) atom adopts a distorted trigonal bipyramidal stereochemistry with an Addison parameter τ value of 0.69. In trigonal bipyramid geometry, the equatorial positions of Cu(II) atom are occupied by three nitrogen atoms (N1,N5,N9) of three pyridine rings of H_5N_{11}-tpm ligand. On the other hand, two nitrogen atoms (N(3) and N(7)) from two pyridine rings coordinate with the Cu(II) ion in the axial positions. The Cu–N distances are well consistent with the corresponding distances of copper complexes with nitrogen-containing heterocyclic ligands. In complex 2, the H_5N_{11}-tpm coordinates to the Cu(II) ion as a pentadentate ligand and acquires, in this case, an anti-anti-anti-anti-anti-syn-syn conformation. The pyrimidine and amine nitrogen atoms of the ligand are not participating in coordination. The observed magnetic moment at 300 K is 1.79 B.M. for the complex of 2, consistent with one unpaired electron in Cu(II) (d9), including a small amount of orbital contribution.

References

[1] J.F. Berry, F.A. Cotton, P. Lei, T. Lu, C.A. Murillo, Inorg. Chem. 42 (2003) 3534–3539.
[2] S.M. Peng, C.C. Wang, Y.L. Jang, Y.H. Chen, F.Y. Li, C.Y. Mou, M.K. Leung, J. Magn. Magn. Mater. 209 (2000) 80–83.

Comparative In Silico Evaluation of Two Hydrazone-Based Derivatives for Their Antiviral Potential Using the AntiVir-Pred Tool

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Abstract

Hydrazone derivatives represent a versatile class of compounds with a wide spectrum of biological activity, including antiviral potential. In this study, two novel hydrazone-based molecules — methyl (Z)-4-(2-methoxy-2-oxo-1-(2-(p-tolyl)hydrazineylidene)ethyl)benzoate and methyl (Z)-4-(1-(2-(3,4-dimethylphenyl)hydrazineylidene)-2-methoxy-2- oxoethyl)benzoate — were evaluated for predicted antiviral activity using the AntiVir-Pred platform. This tool analyzes structure–activity relationships to forecast probable interactions with viral proteins. The first compound exhibited a strong predicted interaction with Dengue virus type 2 genome polyprotein (Pa = 0.6761), followed by moderate affinity for Vaccinia virus DNA polymerase (Pa = 0.2666) and SARS-CoV-2 replicase polyprotein (Pa = 0.1772). The second compound demonstrated a slightly higher affinity towards the same Dengue virus genome polyprotein (Pa = 0.7130), but lower probabilities for other targets, such as Vaccinia virus DNA polymerase (Pa = 0.2411) and SARS-CoV-2 replicase polyprotein (Pa = 0.0672). Overall, while both compounds showed promising interaction profiles against Dengue virus, the first compound exhibited broader antiviral potential across multiple viral targets, including HIV-2 and Coxsackievirus B3. These findings suggest that subtle structural variations, particularly in the hydrazineylidene moiety, influence target specificity and predicted bioactivity. Further experimental studies are required to validate these computational insights.

Table 1. Predicted antiviral activity (Pa values) of two hydrazone derivatives using AntiVir-Pred tool

Target Virus / Protein	Compound 1 *(p-tolyl)*	Compound 2 *(3,4-dimethylphenyl)*
Dengue virus type 2 – Genome polyprotein	0.6761	0.7130
Vaccinia virus (WR strain) – DNA polymerase	0.2666	0.2411
SARS-CoV-2 – Replicase polyprotein 1ab	0.1772	0.0672
HIV-2 – Integrase	0.1707	0.1371
Coxsackievirus B3 – Genome polyprotein	0.0954	0.0771
Infectious bronchitis virus – 3C-like protease	0.0494	0.0350
Dengue virus type 2 (strain Thailand) – NS3 protein	0.0416	0.0247
SARS coronavirus – 3C-like proteinase	0.0136	0.0183

Avocado Seed Waste as Biosorbent of Heavy Metal Ions

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Abstract

Environmental pollution with heavy metals is one of dangerous consequences affecting human health. Heavy metals (e.g. nickel), accumulating in the organism, can damage bone and circulatory system, cause cancer, diseases of liver, kidneys. Considering that they enter the organism with food, it is necessary to develop effective methods for eliminating toxicity of these metals in environment. Sorption is considered as one of the most effective methods for removing heavy metals. Food waste, in particular, avocado seeds (AS) can be used as cheap, accessible and environmentally friendly biosorbents. Our study is aimed at obtaining modified (for increasing sorption efficiency) avocado seed-based sorbents with "memory effect" toward nickel ions in water purification. Structure, properties of synthesized avocado samples were studied using FTIR, XRD, SEM, TGA, DSC analyses.

Crosslinking procedure of powder AS samples was carried out with glycerol and citric acid. FTIR spectra of avocado-based samples were obtained through ATR-FTIR spectroscopy for studying molecular structures, determining functional groups. Powder XRD method of analysis was used for determination of crystallinity, phase, and structural parameters of the synthesized samples. Surface morphology (texture), elemental composition, crystalline structure of avocado-based samples was observed using SEM. Thermoanalytical (TGA/DSC) analyses were used to evaluate the correlation between chemical structure and thermal transitions, stability of avocado-based samples. Sorption experiments were carried out by ICP-MS and titrimetric methods of analysis. Determination of moisture (moisture analyzer MA 50.R Radwag), pH medium (pH-meter Mettler Toledo FE20-Kit FiveEasy^{TM} Benchtop) and solubility (in various solvents) of the powder AS samples were studied as well.

To improve sorption capacity, powder AS samples were crosslinked with citric acid and glycerol. The natural acids present in AS explain medium pH of 6.0±0.2, which is consistent with other studies [1]. It was established that powder AS sample dissolves better in boiling water (26.58%), moisture level (5.97%) of pure AS sample indicated good drying. FTIR and PXRD analyses of modified samples suggested crosslinking and possible complexation reaction between Ni^{2+} ions and functional groups of sorbent. After Ni^{2+} ions sorption SEM analysis showed a rough and coarse morphology of AS sample crosslinked with citric acid, which may be related to the reaction of nickel ions with reactive functional groups on the surface of the sorbent. TGA/DSC analyses showed a decrease in stability of sample crosslinked with citric acid in comparison to pure AS sample. Sorption testing results showed that AS sample crosslinked with citric acid had a relatively high sorption capacity for Ni^{2+} ions compared to other samples and was found to be 92.46 mg/g at pH=7 (vs. 21.8 mg/g for modified AS samples [2]).

There is not much information in the literature about possibility of using AS wastes as biosorbents for heavy metals, so utilization of AS may prove to be a promising, low-cost, sustainable and environmentally friendly direction in the development of new sorbents for water purification. The next stage of research is carried out in the direction of studying the sorption properties of the obtained samples toward Ni^{2+} ions, followed by processing of isothermal and kinetic data.

Keywords: Avocado seed, Biosorbent, Nickel ions.

References

1.Bangar, S., Dunno, K., Dhull, B., Siroha, K., Changan, S., Maqsood, S., Rusu, V.: Avocado see discoveries: Chemical composition, biological properties, and industrial food application. Food Chemistry: X 16, 100507 (2022).

2.Colombo, R., Papetti, A.: Avocado (Persea americana Mill.) by-products and their impact: from bioactive compounds to biomass energy and sorbent material for removing contaminants. A review. International Journal of Food Science and Technology 54(4), 943-951 (2019).

The Effect of Nickel Oxide Nanoparticles on the Properties of Composites Based on Isotactic Polypropylene and Styrene–butadiene Rubber

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Abstract

Thermoplastic elastomers belong to a widely studied group of polymers that have the properties of rubber, while retaining the advantages of thermoplastics in processing. In recent years, increased attention has been paid to composite materials containing nanosized layered silicate or metal-containing fillers, which, even in small quantities (up to 5 wt.%) in the polymer matrix, lead to an increase in the modulus of elasticity, strength, and an increase in the thermal- heat resistance, and combustion resistance of the material [1,2]. In this regard, the use of metal oxide nanoparticles in the production of thermoplastic elastomers based on polyolefins and rubbers in order to improve their physical-mechanical and operational properties is of particular interest.

The objects of the study were thermoelastoplastic compositions based on isotactic polypropylene (PP) and styrene-butadiene rubber (SBR) with 23% of styrene, in a ratio of 50:50. Nickel oxide (NiO) nanoparticles stabilized by a high-density polyethylene polymer matrix were used as a filler. The filler was introduced in amounts of 0.5, 1.0, 2.0 wt.p. Nanocomposite polymer materials were obtained by mixing PP with SBR and nickel–containing nanofiller (NF) on laboratory rollers at a temperature of 165 - 170 ° C for 15 minutes. For mechanical testing, the obtained mixtures were pressed in the form of plates with a thickness of 1 mm at 190 ° C and a pressure of 10 MPa.

The physical-mechanical and thermal properties of the obtained nanocomposites were studied. The introduction of 1.0 mass % of NF into the composition leads to an increase in the strength index (from 8.76 to 16.26 MPa) while maintaining the relative elongation value. An increase in the concentration of NF over 1.0 wt.% leads to a decrease in the strength of the composite (15.17 MPa), which is probably due to the aggregation of nanoparticles, leading to the formation of microdefects in the volume of the polymer matrix. A study of the Vicat softening point of the obtained compositions showed that the introduction of a nanofiller into the PP/SBR composition leads to an increase in the heat resistance index from 113 to 155℃. The melt flow index (at a temperature of 190℃ and a load of 5 kg) of the obtained nanocomposites was studied. It was found that nanocomposites based on PP/SBR do not have fluidity and can be processed only by pressing. The effect of a nanofiller containing NiO nanoparticles stabilized by a polymer matrix of high-pressure polyethylene on the properties of PP/SBR-based composites has been studied. An improvement in the strength and deformation parameters of the obtained nanocomposites has been revealed, which is apparently due to the effect of interfacial interaction of nickel-containing nanofillers in the PE matrix with the components of the PP/SBR polymer composition.

Keywords: isotactic polypropylene, styrene-butadiene rubber, nickel-containing nanofillers.

References

1.Акмырадов А., Ибрагимов М.А., Рахматуллина А.П. Динамические и физико-механические свойства вулканизатов на основе смесей бутадиен-стирольного каучука и функционализированного полимера, полученных жидкофазным совмещением их латексов : OSCXAZ . Ползуновский Вестник, (3), 153–159 (2024).

2.Guliyeva T.M., Kurbanova N.I. Properties of metal-containing nanocomposites on the basis of isotactic polypropylene and butadiene nitrile rubber. High Energy Chemistry 57(2), S60-S64 (2023).

The In Silico Prediction of Antibacterial Activity of α-Keto Acid Aryl Hydrazones

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Abstract

It is well known from the literature that α-keto acid aryl hydrazones are being investigated as biologically active compounds. In our study, we have used the AntiBac Pred program to evaluate the potential antibacterial activity of two synthesized compounds: methyl (Z)-4-(2-methoxy-2-oxo-1-(2-(p-tolyl)hydrazineylidene)ethyl)benzoate and methyl (Z)-4-(1-(2-(3,4-dimethylphenyl)hydrazineylidene)-2-methoxy-2-oxoethyl)benzoate against bacterial microorganisms. In silico analyses performed using the PASS and CHEMBL databases allowed us to assess the potential antibacterial activity of the two synthesized compounds. The predicted activity indicators for various pathogenic microorganisms were analyzed and compared.

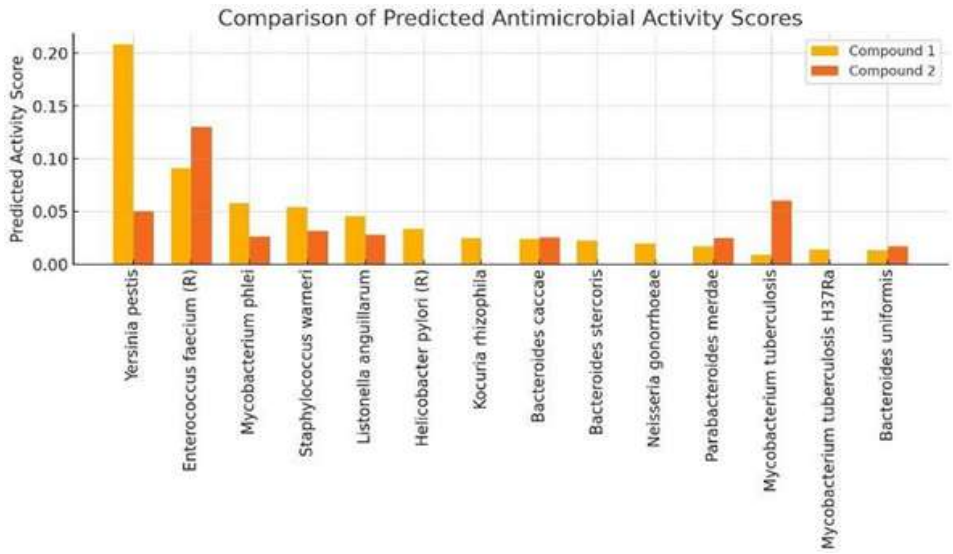

Fig. 1: Graphical Representation of the Predicted Antibacterial Activity of the Compounds.

The analysis of the first compound showed that it exhibited the highest activity against the bacterium Yersinia pestis (score = 0.2086). At the same time, a certain level of activity was also observed against Enterococcus faecium (resistant), Mycobacterium phlei, and Staphylococcus warneri, although these activity levels were generally low (ranging from 0.03 to 0.09). Regarding the second compound, a higher activity score was observed against the resistant strain of Enterococcus faecium (score = 0.1301). This suggests that the compound may have selective potential against multidrug-resistant pathogens. Additionally, weak but notable activity was observed against clinically significant pathogens such as Mycobacterium tuberculosis (0.0603) and Yersinia pestis (0.0502). The predicted activity against other microorganisms for both compounds was recorded at levels of 0.03 or lower, suggesting that their use as broad-spectrum antimicrobial agents may be limited.

Overall, these in silico analyses show that both compounds exhibit selective antibacterial activity and may have potential effects against specific microorganisms. These results could serve as a foundation for the future structural modification of these compounds, potentially improving them into more effective and safer antimicrobial agents.

Obtaining And Studying The Properties Of Nanocomposites Based On A Mixture Of Polyethylenes Of High And Low Pressure With Cobalt-Containing Nano Fillers

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Abstract

It has been investigated the influence of nanofillers addition containing nanoparticles of cobalt oxides, stabilized by the polymer matrix of high-pressure polyethylene, obtained by the mechanical-chemical method, on the peculiarities of structure and properties of the metal-containing nanocomposites on the basis of mixture of high- and low-pressure polyethylenes by the methods of differential-thermal analyses. The obtained results indicate that small quantities of nanofiller (0.3-0.5 mass%) introduced into the polymer, evidently, play the role of structure-forming agents–artificial crystallization nuclei, which favors the appearance of fine spherulite structure in the polymer, characterized by improved physical-mechanical and thermal properties of the obtained nanocomposite.

The development of nanotechnology has opened up the possibility of conducting research in the field of composite nanomaterials and has now made it possible to move on to the creation and use of promising polymer materials for sensors, catalysis, nanoelectronics and having specific physical, mechanical and operational properties: increased thermal and electrical conductivity, high magnetic susceptibility, and the ability to shield ionizing radiation. It is known that the use of d- metal nanoparticles (copper, cobalt, nickel, etc.) in polymers makes it possible to obtain fundamentally new materials that are widely used in radio and optoelectronics as magnetic, electrically conductive and optical media [1,2].

In the work used:- High-pressure polyethylene brand 15803-020, ρ=0.917-0.921g/sm^3 , MFI1.5-2.5 g·10^{-1}min (T=190ºC,load2.16kg);- Low pressure polyethylene brand HM0349PE, ρ=0.949g/sm^3 , MFI 8.3 g·10-1min (T=190ºC,load 21.6 kg). Cobalt oxide nanoparticles stabilized by matrices of low-density polyethylene obtained by the mechanochemical method, were used as a nanofiller. Composition component ratio(wt.%): LDPE/HDPE/LDPE/CoO=50/50/(0.5;1.0;2.0). Nanocomposite polymeric materials are obtained by mixing sequentially HDPE and LDPE and then with a cobalt-containing nanofiller on laboratory rollers at a temperature of 150ºC for 15min. To carry out mechanical tests, the obtained mixtures were pressed in the form of plates 1 mm thick at 190ºC and a pressure of 10 MPa for 10 min.

The physical and mechanical properties of the resulting composites were studied. It was revealed that the best properties are observed in composites containing 1.0 wt.% NF with CoO nanoparticles stabilized by an LDPE matrix, which leads to an increase in the strength index from 16.69 to 20.30 MPa and elongation at break of the composite from 590 to1080 by 1.8 times. The Vicat softening temperature increases from 155°C to 165°C. It has been shown that the activation energy (E_a) of the decay of the thermal-oxidative destruction of the obtained nanocomposite is increased from 232.96 to 268.32 kJ/mol.The improvement in the properties of the composites under study is apparently due to the interfacial interaction of cobalt-containing nanoparticles stabilized by polyethylene matrices LDPE with the components of the mixture of high- and low-density polyethylenes.

Keywords: high pressure polyethylene; low-pressure polyethylene; nanoparticles of cobalt oxide.

References

1. Nikolaychik Yu. A., Kuis D.V., Svidunovich N. A., RovinS. L.: General problems of development and implementation of nanomaterials and nanotechnologies. Casting and metallurgy 4, 152–162 (2020).
2. Kurbanova N.I., MamedovaG.H., GuliyevaT.M., Isgenderova E.G.: Properties of metal-containing composites based on blends of low and high-density polyethylene. Russion Journal of Applied Chemistry8, 801-805(2023).

Prediction of Cardiotoxic Risks of α-Keto Acid Aril Hydrazone Derivatives Based on PASS Online Analysis

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Abstract

In silico analyses conducted via the PASS (Prediction of Activity Spectra for Substances) program platform assessed the potential cardiotoxic effects of two different methyl 4-(2-methoxy-2-oxo-1-(2-phenylhydrazineylidene)ethyl)benzoate derivatives synthesized during the study – methyl (Z)-4-(2-methoxy-2-oxo-1-(2-(p-tolyl)hydrazineylidene)ethyl)benzoate and methyl (Z)-4-(1-(2-(3,4-dimethylphenyl)hydrazineylidene)-2-methoxy-2-oxoethyl)benzoate. The probability of these compounds causing serious cardiotoxic effects such as myocardial infarction was evaluated. For this purpose, the biological activity indicators of each compound, expressed as Pa (Probability of Activity) and Pi (Probability of Inactivity), were analyzed.

For the first compound, the analysis showed Pa = 0.283 and Pi = 0.242. This result indicates that the potential for myocardial infarction is low, though not entirely excluded. The closeness of the Pa and Pi values suggests that the effect is uncertain and the likelihood of occurrence is weak. For the second compound, the predicted values were Pa = 0.317 and Pi = 0.167. These values indicate that the second compound has a higher cardiotoxic potential compared to the first one. Specifically, the Pa value significantly surpasses the Pi value, indicating a higher probability of the effect occurring.

Overall, the assessment indicates that while the risk of myocardial infarction is low for both compounds, it is more prominent for the second compound. Therefore, further research is recommended, particularly to explore the toxicological properties of these compounds through in vitro and in vivo testing to refine their cardiotoxicity profiles. If potential toxic effects are confirmed, structural modifications and optimization of functional groups to synthesize safer derivatives would be advisable.

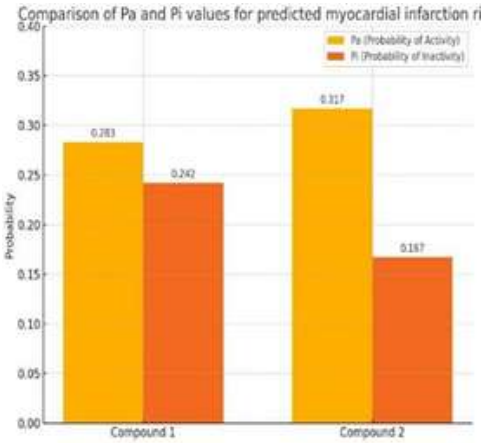

Fig. 1: Graph of the probability of myocardial infarction for the compounds.

Biodiesel Production from Waste Cooking Oil with Heterogeneous Green Catalysts

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Abstract

Fossil fuels provide 90% of global energy, with fuel accounting for 81% of total consumption [1]. But due to the environmental impacts of fossil fuels and fading resources, the search for sustainable substitute has been significantly increased. Among the green energy choices, biodiesel excels for its renewability and biodegradability. Biodiesel is produced through transesterification reaction, which occurs between oil and alcohol with the help of a catalyst [2]. While homogeneous catalysts are proven to be sufficient, heterogeneous catalysts have much better sustainability and feasibility features. For this reason, heterogeneous catalysts, particularly those produced from biomass, have attracted attention. This research paper studies pomegranate and banana peel ash catalysts while optimizing reaction time, alcohol-to-oil ratio, and temperature to find the best yield of biodiesel.

Banana and pomegranate peels were turned to ashes at a furnace under 700C for 3 hours. Using those peel ash catalysts, transesterification reaction conducted in round bottom flask setup. Reaction was repeated several times with both ethanol and methanol, while maintaining reaction temperature at 50-60C and 3.5-4.5h reaction time. After the reaction, biodiesel floated above glycerin due to having lesser density, while catalyst ash precipitated. The mix was separated using a centrifuge. Catalysts and biodiesel were analyzed using Scanning Electron Microscope (SEM) and Fourier-Transform Infrared (FTIR) spectroscope to prove the existence of methyl (ethyl) ester groups.

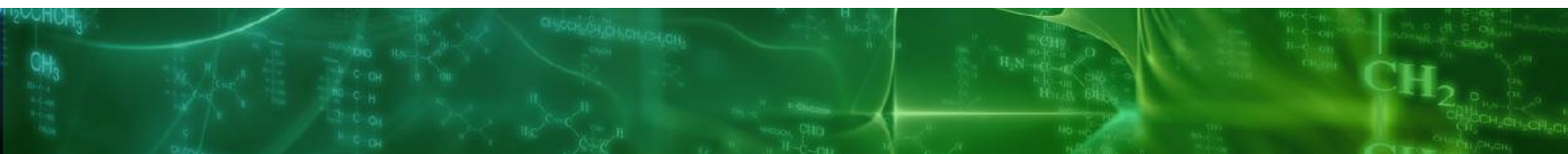
Several tests were conducted to analyze the properties of obtained biodiesel and green catalyst. Catalyst's microporous structures were defined by SEM analysis method. FT-IR spectroscopy helped to prove the existence of methyl ester groups in obtained sample of biodiesel. As one of the most important data, properties of biodiesel were defined and checked according to ASTM standards. Among the impactful ones are: density (0.8 g/cm^3), kinematic viscosity (3.7 cSt), and flash (lowest temperature of ignition) point (132C). Conversion of biodiesel was higher than 90% when waste cooking oil had been transesterficated with methanol, while with ethanol this number was drastically lower.

This research concludes that agricultural wastes such as banana and pomegranate peels can play vital role for biodiesel production. Thus, the benefits of biodiesel production are not limited to recycling waste cooking oil, which reduces waste and costs, but also include recycling green waste. Usage of biomethanol would make this production even more ecologically viable. To get the maximum benefits, the awareness about recycling oil and biowastes should be raised among the people.

Keywords: Biodiesel, Waste Cooking Oil, Green Catalyst.

References

1. Ahmed I. Osman, et al: Cost, environmental impact, and resilience of renewable energy under a changing climate: a review. Environmental Chemistry Letters 21, 741-764 (2023)
2. R. Nayab, et al: Sustainable biodiesel production via catalytic and non-catalytic transesterification of feedstock materials – A review. Fuel 328, article 125254 (2022)



Comprehensive Analysis Of Electrical Conductivity In Diesel Fuel Enhanced By The Integration Of Synthesized Aminoester-Based Additives Into Diesel Distillates

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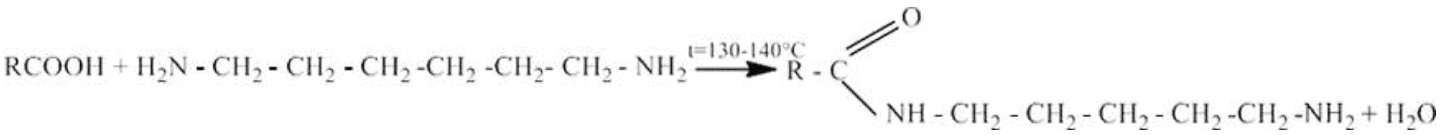
Abstract

The baseline electrical conductivity of untreated diesel fuel was determined to be 95 pS/m after one day, decreasing to 77 pS/m after prolonged storage periods of 10, 20, and 30 days. Conversely, the introduction of synthesized aminoester compounds, derived from cottonseed fatty acid and diethylenetriamine, as antistatic agents at concentrations of 0.05%, 0.1%, and 0.15% led to a marked enhancement in conductivity. Specifically, the electrical conductivity of the treated diesel fuel was observed to increase to 4090 pS/m, 5110 pS/m, and 10,000 pS/m, respectively, following a 40-day storage period.

The accumulation of static electricity during the processing and transportation of crude oil and petroleum products presents significant hazards, including the potential for fires and explosions. To mitigate these risks, the implementation of specialized safety protocols and advanced technological solutions is essential. Such measures not only safeguard operational safety but also protect critical equipment from damage. In light of these considerations, extensive experimental investigations have been conducted to address the challenges of electrification in this domain.

Amidoesters were synthesized using a 1:1 molar ratio of fatty acids derived from sunflower, corn, cottonseed, soybean, and palm oils with monoethanolamine and diethylenetriamine as reactants. The resulting amidoester compositions were incorporated into diesel distillate as antistatic additives at concentrations of 0.05%, 0.1%, and 0.15%. The electrical conductivity of the treated diesel fuels was subsequently evaluated to assess the effectiveness of these additives.



The electrical conductivity of diesel fuel was significantly enhanced upon the addition of synthesized amino esters as antistatic additives to the diesel distillate at concentrations of 0.05%, 0.1%, and 0.15%.

Sample Names	Solvent Concentration, %	Electrical Conductivity, Ps/m			
		After 1 Day	After 10 Days	After 20 Days	After 30 Days
Aminoester derived from sunflower fatty acid and diethylenetriamine in a 1:1 molar ratio	0,05	598	820	1350	1450
	0,1	1740	2035	2280	2300
	0,15	3020	3225	3450	3530
Aminoester derived from corn fatty acid and diethylenetriamine in a 1:1 molar ratio	0,05	463	620	902	1250
	0,1	630	820	1240	1550
	0,15	730	1200	1880	1980
Aminoester derived from soybean fatty acid and diethylenetriamine in a 1:1 molar ratio	0,05	4210	4235	4250	4280
	0,1	4245	4285	4320	4380
	0,15	4290	4330	4440	9010
Aminoester derived from cotton fatty acid and diethylenetriamine in a 1:1 molar ratio	0,05	1235	1470	2350	4090
	0,1	4055	4690	4920	5110
	0,15	8220	8227	8228	10000

As observed in the table, the amidoester composition derived from cotton fatty acid and diethylenetriamine exhibits a more pronounced antistatic effect compared to amidoester compositions based on other vegetable fatty acids.

Keywords: aminoester, fatty acid, diesel fuel, additive.

References

1. Putko, A.E., Kitsis, S.I. Physical foundations of the phenomenon of oil electrification in oilfield pipes. Materials of the International Scientific and Technical Conference dedicated to the 40th Anniversary of Tyumen State Oil and Gas University, Tyumen: Tyumen State Oil and Gas University, 2003, Vol. 2, pp. 91-92.

2. Abdullaeva, N.R., Ismailov, T.A., Mamedova, T.A., Magerramov, R.C., Veliev, K.R., Abbasov, V.M. Synthesis and research of antistatic additives to diesel fuels based on petroleum acids. Processes of Oil Chemistry and Oil Refining, 2011, Vol. 12, No. 3 (47), pp. 168-177.

3. Vlasova, E.P., Kitsis, S.I. Investigation of the influence of oil parameters and pipeline parameters on the process of electrification of oil. Izvestiya Uzov. Oil and Gas, 2007, No. 4, pp. 87-93.

Synthesis of a Novel Schiff Base Containing a 2-phenyl-2H-chromene-3-carbaldehyde Scaffold

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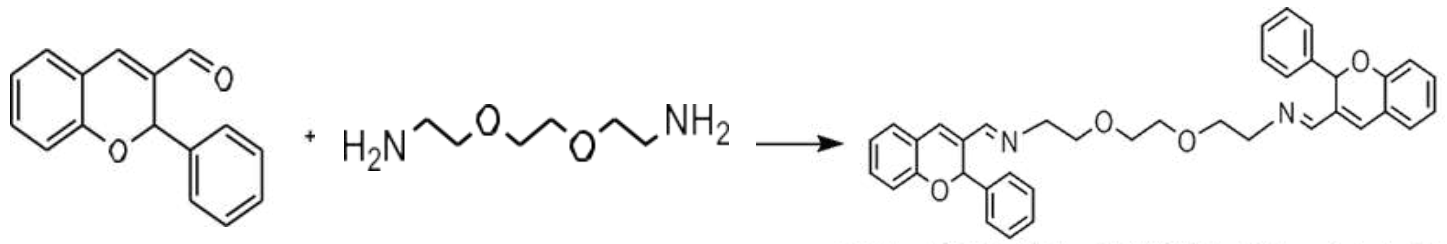
Abstract

The chromone moiety is an important part of the pharmacophores of several naturally occurring and synthetically produced biologically active compounds. Many of them are still under investigation by synthetic, organic, and medicinal chemists because of their useful medicinal applications. Recently, there has been an increasing interest in combining the chromene scaffold with Schiff bases.

Schiff bases are bioactive substances that are generated through the condensation of a primary amine with a carbonyl compound. The special function of the imine bond in Schiff bases is to confer on these substances' extensive biological activity. The electrophilic carbon and nucleophilic nitrogen present in the imine bond offer vast binding possibilities to different nucleophiles and electrophiles, which helps in the inhibition of specific diseases, enzymes, or DNA replication.

Taking into account the above-mentioned, we synthesized a novel hybrid molecule that contains chromene and Schiff base moieties. For this purpose, we performed the reaction between 2-phenyl-2H-chromene-3-carbaldehyde and ethylene glycol bis(2-aminoethyl) ether, and as a result of this reaction, we received a novel Schiff base, which is called N,N'-((ethane-1,2-diylbis(oxy))bis(ethane-2,1-diyl))bis(1-(2- phenyl-2H-chromen-3-yl)methanimine). For this, to a solution of prepared 2-phenyl-2H-chromene-3-carbaldehyde in a round-bottom flask, ethylene glycol bis(2-aminoethyl) ether was added under continuous stirring. Upon reaction completion, the reaction solution was poured onto ice. After ice melts, the formed white precipitate is easily filtered with water and left to dry. The drying sediment changed its color to burnt orange.



The formation of the product was confirmed by 1H and 13C NMR spectroscopy methods. According to the 1H NMR spectrum, it was observed that the signal from the aldehyde group in the initial compound, which is observed at 9.33 ppm, fully disappeared; instead of it, we observed the signal from the imine bond at 8.02 ppm. The same signal at the 13C NMR spectrum was observed at 161.13 ppm. Along with it, the signal of 2NCH2 appeared at 61.29 ppm, whereas the signals of CH2-O appeared at 70.53 and 70.62 ppm, respectively.

Finally, the biological activity of the synthesized compound was investigated against gram-positive and gram-negative strains of bacteria, and as a result, it was compared with the data of the standard antibiotic- ampicillin. The obtained results allow us to conclude that the synthesized Schiff base demonstrates better activity in comparison with the pristine antibiotic.

Keywords: Schiff Bases, Chromene Scaffold, Biological Activity.

References

1. Johnson, T. A., Roe, E. W., Crawford, M. J., Basile, O. N., Shellenberger, B. M., Rudolph, M. E., ... & Henry, G. E. Synthesis, antioxidant, dna interaction, electrochemical, and spectroscopic properties of chromene-based schiff bases: Experimental and theoretical approach. Journal of Molecular Structure, 1307, 138020 (2024).

2. Khan, K. M., Ambreen, N., Hussain, S., Perveen, S., & Choudhary, M. I. Schiff bases of 3-formylchromone as thymidine phosphorylase inhibitors. Bioorganic & medicinal chemistry, 17(8), 2983-2988 (2009)

3. Mermer, A., Demirbas, N., Uslu, H., Demirbas, A., Ceylan, S., & Sirin, Y. Synthesis of novel Schiff bases using green chemistry techniques; antimicrobial, antioxidant, antiurease activity screening and molecular docking studies. Journal of Molecular Structure, 1181, 412-422 (2019).

4. Nayak, S. G., & Poojary, B. Synthesis of novel Schiff bases containing arylpyrimidines as promising antibacterial agents. Heliyon, 5(8) (2019).

Innovative approaches in Chemical Engineering for Cancer treatment

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Abstract

Recent improvements in chemical engineering have led to new methods for treating cancer. Traditional treatments like chemotherapy and radiation can cause many side effects because they are not very targeted. With better knowledge of cancer biology, especially the tumor environment and genetic factors, researchers have developed more precise treatments. This paper shows how chemical engineering helps to create improved drug delivery systems, new nanomaterials, and better bioprocessing techniques to treat cancer more effectively.

This paper reviews recent studies that combine chemical engineering with cancer treatment. It focuses on research about nanoparticle-based drug delivery, the use of biomaterial scaffolds to change the tumor environment, microfluidic devices for personalized therapy, and bioreactor techniques for largescale production of cell and gene therapies. The review also includes historical developments in cancer treatment to show how these new methods have evolved.

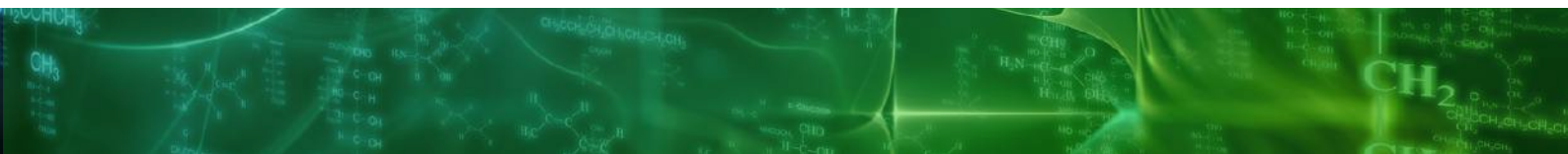
The review shows that nanoparticles made from polymers and lipids can improve how cancer drugs are delivered, making them more effective and reducing side effects. Microfluidic devices have helped in creating personalized treatment plans by mimicking the conditions inside tumors. Advances in bioreactor technology have improved the production of cell and gene therapies, making these treatments more practical for clinical use. Together, these engineering techniques allow for more precise targeting of cancer cells.

Chemical engineering now plays an important role in developing new cancer treatments. By using advanced drug delivery systems, innovative biomaterials, and efficient production methods, these advances can lead to better outcomes for patients. Ongoing research and collaboration between engineers and medical scientists are essential to bring these promising treatments into everyday clinical practice.

Keywords: cancer, chemical engineering, cancer treatment, drug delivery systems, tumor.

References

1. Si-Shen Feng, Shu Chien. (2003). Chemotherapeutic engineering: Application and further development of chemical engineering principles for chemotherapy of cancer and other disease
2. Torchilin, V. P. (2014). Multifunctional, stimuli-sensitive nanoparticulate systems for drug delivery. Nature Reviews Drug Discovery



Development of a Sustainable Hybrid Catalyst NaOH/CaO Derived from Eggshell Waste for Biodiesel Production

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Abstract

The increasing environmental impact of fossil fuels has necessitated the development of renewable energy sources, such as biodiesel, which is composed of fatty acid methyl esters (FAME). The efficiency of biodiesel production heavily depends on the catalytic systems used in the transesterification process. Traditional homogeneous catalysts (e.g., NaOH) face limitations such as non-reusability and high costs, while heterogeneous catalysts (e.g., CaO) often require optimization to achieve competitive yields. This study focuses on the development and optimization of a hybrid NaOH/CaO catalyst to enhance biodiesel production from waste cooking oil (WCO). The CaO component of the catalyst was synthesized from calcined chicken eggshells, a sustainable and cost-effective source, while the hybrid catalyst was prepared in both solid and solution-based forms with varying NaOH-to-CaO ratios. The primary objective was to optimize the catalyst's performance and compare the properties of the produced biodiesel against international standards, namely ASTM D6751 and EN 14214. The highest biodiesel yield of 91% was achieved using a 1:1 CaO-to-NaOH solution-based catalyst at a 3% loading. Increasing the catalyst concentration to 6% further improved the yield to 94.8%, demonstrating the catalyst's efficiency. However, reducing the methanol-to-oil ratio to 1:6 resulted in a lower yield of 82.8%, indicating the importance of methanol content in the transesterification process. The biodiesel produced met the ASTM D6751 and EN 14214 standards, with key properties such as density, viscosity, and acid value falling within the specified ranges. The study also compared the performance of the hybrid catalyst with individual NaOH and CaO catalysts. The hybrid catalyst outperformed both, achieving higher yields under the same conditions.This suggests that the combination of homogeneous and heterogeneous properties in the hybrid catalyst enhances its catalytic activity, making it a promising alternative for biodiesel production. Future research will focus on optimizing glycerin separation for applications in pharmaceuticals, cosmetics, and bioplastics. Advanced characterization techniques, such as XRD, GC, and FTIR, will be employed to further analyze the catalyst's structure and the biodiesel's composition. Additionally, the study aims to explore sustainable methanol synthesis and recovery methods to create a more eco-friendly production system. Alternative biogenic CaO sources, such as oyster shells, will also be investigated to further reduce the environmental impact of biodiesel production. In conclusion, this study demonstrates the potential of a hybrid NaOH/CaO catalyst derived from eggshell waste to improve biodiesel yield and quality, offering a sustainable and efficient alternative to traditional catalysts. The findings pave the way for further research into optimizing the biodiesel production process and exploring new biogenic sources for catalyst development.

Keywords: Eggshells,Hybrid catalyst, Biodiesel,WCO, transesterification.

References

1.Hangun-Balkir, Y., "Green Biodiesel Synthesis Using Waste Shells as Sustainable Catalysts with Camelina sativa Oil," Journal of Chemistry, vol. 2016, pp. 1-10, 2016.

2. H. Hadiyanto , Asha Herda Afianti , Ulul Ilma Navi'a , Nais Pinta Adetya , W. Widayat , Heri Sutanto , The development of heterogeneous catalyst C/CaO/NaOH from waste of green mussel shell (Perna varidis) for biodiesel synthesis, Journal of environmental chemical engineering, vol. 5,no. 5,Oct. 2017.

3. Adeyemi, D. T., Saleh, A., Akande, F. B., Oniya, O. O., & Ola, F. (2024). Determination of Fuel Properties of Biodiesel from Sand Apple Seed Oil with Automotive Gas Oil Blend. Journal of Applied Sciences and Environmental Management.

Biodegradable Flocculating Agents Based on Polyaspartamide Derivatives

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Abstract

Cationic and anionic polymers can be applied as biodegradable flocculants in wastewater treatment processes. Within this article, the synthesis and application of two polymers, namely anionic polysaspartic acid sodium salt (PASP-Na) and cationic polyaspartamide modified with cysteamine (CEA) have been discussed. The cationic polymer, PASP-CEA-DETA was prepared through thiolation utilizing CEA in order to produce short thiolated side groups. The stability of the cationic polymer PASP-CEA-DETA has been tested through various pH levels. Results demonstrated high stability at lower pH levels, with the figure for over 12 days at pH 5, steadily diminishing to over 2 days at pH 12, which indicates that PASP-CEA-DETA is more stable in acidic conditions. With the help of spectroscopy, the cationic nature of the polymer was confirmed. Within acidic conditions, the polymer demonstrated effective flocculation, as a result of which the turbidity of the kaolin solution was reduced by 98.9%. The implementation of the cationic polymer was also approved via charge analysis and turbidity measurements. In addition, the chemical oxygen demand test was conducted in order to display polymer efficiency within coagulation. An anionic flocculant also showed enhanced performance in alkaline conditions by interacting with positively charged particles which eventually confirms its anionic nature.

Keywords: polysuccinimide, polycondensation, flocculation, thiolation, biodegradation, polyaspartamide.

References

1. A. Wibowo, M.A. Marsudi, E. Pramono, J. Belva, A.W. Parmita, A. Patah, et al., Recent improvement strategies on metal-organic frameworks as adsorbent, catalyst, and membrane for wastewater treatment, Molecules 26 (17) (2021) 5261.
2. A. Mammadova & Gyarmati, Benjámin & Sárdi, Kitti & Paudics, Adrien & Varga, Zoltán & Szilágyi, András. (2022). Thiolated cationic poly(aspartamides) with side group dependent gelation properties for the delivery of anionic polyelectrolytes. Journal of Materials Chemistry B.
3. E.M. Ahmed, Hydrogel: Preparation, characterization, and applications: A review, J. Adv. Res. 6 (2) (2015) 105–121.
4. C.Y. Teh, P.M. Budiman, K.P.Y. Shak, T.Y. Wu, Recent advancement of coagulation– flocculation and its application in wastewater treatment, Ind. Eng. Chem. Res. 55 (2016) 4363–4389.
5. D. Liu, S. Zhou, Application of chemical coagulation to phosphorus removal from glyphosate wastewater, Int. J. Environ. Sci. Technol. 19 (2022) 2345–2352
6. C. Zhang, S. Wu, J. Wu, D. Wu, X. Qin, Preparation and characterization of microporous sodium poly(aspartic acid) nanofibrous hydrogel, J. Porous Mater. 24 (2017) 75–84.
7. E.M. Ahmed, Hydrogel: Preparation, characterization, and applications: A review, J. Adv. Res. 6 (2) (2015) 105–121
8. H. L. Zheng, Y. J. Sun, J. S. Guo, F. T. Li, W. Fan, Y. Liao, Q. Q. Guan, Synthesis and characterization of hydrophobically associating cationic polyacrylamide, Ind. Eng. Chem. Res. 2014, 53, 2572.

Efficient Plasticizers for Polyvinyl Chloride

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Abstract

This thesis is devoted to the production and study of effective and environmentally friendly plasticizers using heterogeneous catalysts.

Esters of aliphatic, alicyclic, and aromatic carboxylic acids are promising chemical products with wide practical use in various industrial fields as plasticizers. Plasticizers are among the most important classes of polymer additives that improve the plasticizing properties of materials. Since plasticizers are widely used in the production of consumer goods, it is important to consider their effects on human health. Currently, the use and market of plasticizers are under strict control of environmental and health protection directives. According to research, products made of PVC with the plasticizer dioctyl phthalate (DOP) are harmful to health, leading to bans on the production and sale of children's toys and some household items made from these materials [1].

We developed single-stage processes for obtaining esters of carboxylic acids using a heterogeneous catalyst (ZnO, TiO_2 (+FemOn)) and proposed a basic technological scheme [2]. Due to the advantages of carboxylic acid esters and to increase the range of effective, eco-friendly plasticizers, in this study we synthesized them from individual aromatic, aliphatic and alicyclic, natural, and synthetic petroleum-based carboxylic acids with alcohols in the presence of a heterogeneous catalyst. The synthesis was conducted in a reaction flask equipped with a mechanical stirrer, reflux condenser, water separator, and thermometer. The acid and an excess of alcohol (30%) were reacted in an organic solvent in the presence of heterogeneous catalysts until water release ceased. The physical and chemical parameters of the synthesized esters were determined to GOST 8728-88 standards.

Besides suitable properties, a plasticizer must be well compatible with the polymer matrix. Therefore, the mixtures were thermostated for 3–6 hours at 65, 75, and 85°C until complete swelling of the PVC composition in the plasticizer. The mixtures were cooled to room temperature and held under load until greasy spots disappeared on filter paper, after which the optimal compatibility limit of the synthesized esters with PVC (30–40 parts by mass) was determined. Compositions with synthesized esters matured within 0.25–6 hours, while those with DOP matured in 8 hours, indicating better compatibility of the synthesized diesters with PVC compared to DOP.

The proposed synthesis scheme reduces the steps of neutralization, washing, and drying of the target products in accordance with global manufacturing standards, and significantly reduces corrosion in metal equipment and reactors. The scheme is distinguished by not requiring additional disposal of acidic and alkaline waste from the esterification process that uses acid catalysts. The use of heterogeneous catalysts simplifies the technology, thus ensuring environmental cleanliness.

Keywords: carboxylic acids, esterification, catalyst, plasticizer, polyvinyl chloride.

References

1. Fundamentals of Plasticizer Production: A Textbook / S.N. Lakeev, I.O. Maydanova, O.V. Ishalina. – Ufa: UGNTU Publishing House, 2015. – 162 p.
2. S.A. Isgandarova, L.M. Efendiyeva, G.G. Nasibova, Y.P. Cherepnova, E.M. Guliyeva, Sh.R. Mamedova. Development of eco-friendly technology for obtaining complex esters / Republican Scientific Conference dedicated to the 80th anniversary of Honored Scientist Akif Hamid oglu Azizov, November 15, 2023, p. 135