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رشت ، دانشگاه گیلان
۱۴ الی ۱۶ مهرماه ۹۴

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University of Guilan . Rasht . 6-8 october 2015

2nd Iranian Student Chemistry Conference
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Prediction of nasal pungency thresholds of volatile organiccompounds based on ant colony optimization algorithm

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Abstract:

Volatile organic compounds are major contaminants, degrading air quality in both indoor and outdoor environments.[1] In this paper, multiple linear regression (MLR) and the novel feature selection method of ant colony optimization (ACO) algorithm,[2,3]were employed to select the optimal subset of descriptors that have significant contribution to nasal pungency thresholds (NPTs) of a group ofvolatile organic compounds. Artificial neural network (ANN) technique was used for modeling NPTs values of the desired compounds.

In the first step of the study, six variables including information indices and RDF, GETAWAY, geometrical and 3D-Morse descriptors were selected by MLR. The descriptors were considered as inputs for the artificial neural network to develop an accurate model. The results showed that a 6-8-1 back-propagation neural network trained by Levenberg–Marquardt algorithm with tansig/purelin activation functions for the hidden and output layers gives a relatively good model.

The nonlinear model had root mean square error (RMSE) of 0.14 for training set, o.17 for test set and 0.31for validation set. Application of ACO algorithm resulted in selection of just three variables belonged to topological and 3D-Morse descriptors. Again, the descriptors were employed for nonlinear modeling by ANN technique. The model developed by a 3-5-1 neural network gave the statistics of RMSE=0.00011 for training set, RMSE=0.00013 for test set, and RMSE=0.00024 for validation set. Significant decrease in the error values obtained by combination of ACO and ANN showed superiority of ant colony feature selection algorithm over multiple linear regression formodeling of nasal pungency thresholds of the volatile organic compounds. Results of the study suggest to use theACO algorithm as an efficient feature selection method fordevelopinghigh quality models for prediction of nasal pungency thresholdsof other classes ofchemicalcompounds.

Keywords: Nasal pungency thresholds, Modeling, Feature selection, Ant colony optimization, Artificial neural network.

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Proton transfer reaction in the ground and excited states of naphthalene-fused analogs of 2-(2'-hydroxyphenyl) benzimidazol

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Abstract:

Proton transfer is one of the most fundamental reactions in chemical and biological sciences.[1,2] The various types of proton transfer reactions have been reported in both the ground and excited states.[3] Intramolecular proton transfer (ESIPT) has received much attention because of the simplicity of its reaction pattern. The ESIPT system generally requires hydrogen bonding (H-bonding) formation between vicinal proton-donor groups and proton-acceptor groups.[4,5] In this study, intramolecular proton transfer in the ground (GSIPT) and excited (ESIPT) states of naphthalene-fused analogs of 2-(2'-hydroxyphenyl) benzimidazol (HBN) were investigated using DFT method (PBE1PBE) in conjunction with the 6-311++G(2d,2p) basis set of theory by using the Gaussian 09 software.[6,7] Although, the ground state intramolecular proton transfer in the studied species is not possible because of the high energy barrier and high instability of the keto form (K-form) with respect to the enol one (E-form), nevertheless, photoexcitation from S_0 to S_1 state stimulate the operation of the ESIPT process. The PT process is shown in Figure 1. The results show that, negative charge of oxygen atom and positive charge of H atom during OH···N to O···HN PT reaction increases.

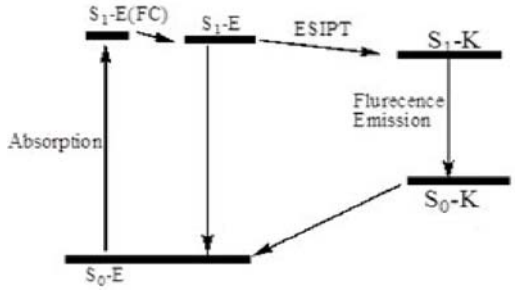

Figure1. PT process in HBN

Keywords: GSIPT; ESIPT; PBE1PBE; HBN.

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Interaction of hexagonal boron nitride nanosheet with silicon cluster: a theoritical of study

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Abstract:

By performing density functional theory calculations, we investigate the structural and electronic properties of Si6 cluster with hexagonal boron nitride nano sheet (h-BNNS) in several states (T1,T2 and T3). We found that interaction of Si_6 cluster with h-BNNS lead to decrease in its electronic band gap, albeit to different magnitudes varying 2.149, 2.095 and 2.204 eV depending state deposition (T1, T2 and T3). Interaction energy for states T1, T2 and T3 is -3.206, -3.202 and -3.332 eV, respectively. The more stable configuration is while Si6 placed on top of nitrogen atom on h-BNNS (state T3). The obtained results suggest that the h-BNNS may be potentially used in Si6 cluster sensor applications.[1-7]

Keywords: Boron nitride, Silicon, Cluster, DFT, Nanosheet.

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Encapsulation of Thalidomide stereoisomers in cucurbit[8]uril as a molecular container for drug delivery: a computational study

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Abstract:

Thalidomide was presented in october 1957 by the German company Chemie Grunenthal as a "safe" sedative/tranquilizer, but It's using was stopped because of the side effect on birth defects.[1] Recent evidences indicate that thalidomide has significant effects on the treatment of diseases such as erythema nodosum leprosum (ENL), severe mucosal ulcers (*e.g.*, associated with HIV infection or Behçet's disease), lymphocytic skin infiltrations, cutaneous lupus erythematosus and chronic graft-versus-host disease.[1] It also used for conditions including some symptoms of HIV/AIDS, Crohn's disease, sarcoidosis and rheumatoid arthritis and also improves symptoms of multiple myeloma.[2] Thalidomide is a highly toxic drug, so long-term use of this medication cause peripheral neuropathy. According to this fact, efforts to reduce the side effects of this medicine are ongoing.[3]

Mock *et al*. in 1981, named the macrocyclic methylene-bridged glycoluril hexamer (CB[6]) Cucurbit due to its resemblance to the cucurbitaceae. Then the other compounds of cucurbit family have been synthesized (CB[5]–CB[10]). Shape, solubility and chemical functionality make these compounds suitable for molecular recognition and nanotechnology.[4] Cucurbit as a kind of molecular containers with high affinity has essential features to be used in drug delivery. Encapsulating drugs not only increases drug stability but also reduces the unwanted side effects of drugs. These results demonstrate that cucurbits as nano cavity can be useful in advanced drug delivery.[5]

In this work, we performed an initio studies on the stabilities and structural, as well as, electronic properties of the complex formation of CB[8] with two stereoisomers of thalidomide. The geometry optimization was performed for all structures, using the B3LYP/3-21g. Single point energy calculations carried out using the density functional theory method B3LYP with the standard 6-31G(d,p) basis set. The calculations show interesting structural features and stability orders. Results reveal good absorbing energy, the frontier orbital graphics and electrostatic potential surfaces confirms the good capsulation of drug. This capsulation protects brain from the neurotoxicity effects of the talidomide. The results and various aspects of these calculations will be presented in detail and discussed.

Keywords: Thalidomide, Cucurbit[8]uril, DFT, Drug delivery

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Removal of lead (II) ionsfrom aqueous solutions using local plant of Guilan province: Eryngiumcampestre(Choochagh)

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Abstract:

Lead is recognized as a longstanding environment contaminant. It can be found inwastewater generated by various industries such as acid battery, ceramic and glass manufacturing, metal planting and finishing, printing, tanning, and production of lead additives for gasoline. The efforts on reducing lead concentration in the effluent wastewaters are motivated by the toxic effects of lead on the aquatic world and the risk of contamination of water resources designated for human consumption. Current USEPA drinking water standard for lead is 0.015 mg/l.[1]

Acute lead poisoning in humans causes severe damage to the kidneys, liver, brain, and nervous system while a long term exposure may induce sterility, abortion, and neonatal death.[2]The removal of such a harmful ingredient from the water bodies became unavoidable. The most widely used techniques to remove lead from wastewater include ion exchange, chemical coprecipitation, reverse osmosis, evaporation, membrane filtration and adsorption.[3]

Adsorption onto plants were found to be a promising technique as it enables the removal of noticeable amounts of lead from solutions. In the present study, a deeper understanding of adsorption behavior of Pb(II) from aqueous systems onto Eryngium Campestre (EC) plant has been attempted. Results showed a great amount of adsorption (95 % adsorption) using the plant. Sorption capacity and effect of different parameters like optimum pH, dose of absorbent, contact time between absorbent and Pb(II) solution were measured.

Keywords: Lead (II), Adsorption, Eryngium Campestre (EC), Sorption Capacity.

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Use of image processing as new method for calculate mixing time in stirred tanks

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Abstract:

Mixing is a critical process in chemistry because the quality of the final product and its attributes are derived by the quality of the mixing process.[1] Fluid mixing with stirred vessels are widely used in the chemical, petrochemical and cosmetic industries for the production of liquid dispersions and emulsions.[2]

The knowledge of mixing time is one of the fundamental importance for mixing investigation in agitation systems.[3] In fact, this characteristic controls the performance of the mechanically agitated tanks and has a direct influence on the cost of the agitation process.[4] Determine of mixing time with new methods is important so in this paper, the image processing as new method was used to calculate the mixing time.[5] The method involves colorimetric diagnosis of digital images, deduced from a video captured during the mixing process.[6] The advantages of this method are: (1) there is no disturbance of the fluid flow, (2) it covers all parts of stirred tank and (3) measuring and determination of the degree of homogeneity is relatively effortless and cheap since it requires only a standard camera and commercial software for digital image analysis. For each experiment, a pulse of tracer is added to the liquid bulk. Mixing time is typically considered as the time required for the tracer concentration to reach within 95% of the completely mixed value (t_{95}) i.e. the time whichtakes for the fluctuationof the bulk concentration to be below 5%of the concentration achieved at perfect mixing.[7] In this study the affecting parameters on mixing time in a fixed geometrical condition have investigated by impellers rotational speed N (rpm) and concentration measuring location. Water as a Newtonian fluid and concentrated solution of colour material hasbeen used as a processing fluid and a tracer, respectively. The experimental results showed that, unlike the power consumption, the mixing time decreased by increasing the impellers rotational speed. The variation of mixing time versus the concentration measuring locations is decreasingly. The experimental results showed that, mixing time decreased by increasing distance between measuring point and the wall of the tank.

Keywords: Stirred tank, Mixing time,Image processing, Colorimetric method, Newtonian fluid, Turbine Rushton disc.

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Environment and substituent effects on the electronic absorption spectra of some azoquinoline dyes

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Abstract:

Hydroxy azo dyes are the most widely used class of coloring materials due to their massive application in various fields of science and technology. They are mainly used for coloring substrates in biological and medical studies and in the field of non-linear optics and optical data storage devices.[1] Many studies have been dedicated to synthesis and spectroscopic characterization of these dyes for improving their photophysical and photochemical features.[2] The azo-hydrazone tautomerism of hydroxy azo compounds and effect of tautomerism on their photophysical properties has been known for many years and was reviewed several times.[3] The azo-hydrazone tautomerism is described by the intra-molecular proton transfer between the phenol and imine groups in ground and/or excited state. This process leads to rearrangement of the electronic density in the molecule. In general, type of solvent, substituents structure and pH are the most important factors, which greatly influence the photophysical and photochemical properties of the azo-hydrazone compounds.[4]

The solvent effect can be determined by solvent polarity scale or solvatochromic parameters.[5] The solvent characteristic is very important factor in formation of the tautomers and their stability in solutions. In fact, the state of azo-hydrazone equilibrium in solution is closely related to the nature and degree of intermolecular interactions. In general, hydrazone form is favored by polar media, and by electron-withdrawing substituents in the conjugated phenyl ring. This arises from a relatively large dipole moment changes during transition from azo to hydrazone form that is stabilized in more polar solvents.[6] Azo-hydrazone tautomerism has been studied by various optical techniques, including electronic method. Due to the characteristic differences between the optical spectra of the dyes in azo and hydrazone forms, azo/hydrazone tautomeric behavior can be investigated from the electronic spectra. Therefore, electronic spectroscopy is one of the most applicable and successful techniques for investigating the azo/hydrazone tautomerism. Spectroscopic methods, based on absorption spectra, give valuable information on contribution of different types of solute–solvent interactions using multi-parameter solvent polarity scales.[7]

In this work, the spectroscopic properties of some azoquinoline compounds in various organic solvents with different polarities and polarizabilities were studied at room temperature. The azoquinoline dyes investigated in this work possesses the electron-withdrawing and electron donor groups attached to the phenyl ring. Therefore, this report also concerns the substituent effect on the spectral and tautomeric properties of the dyes. Moreover, a detailed quantitative study was carried out on the nature and extent of solvent-solute interactions using correlations with multi-parameter solvent polarity scales. Such information is essential for design of new azo

derivatives where one of the tautomers is preferentially dominant depending on the host environment. The work reported here also provides information about the effect of anisotropic medium on azo-hydrazone tautomerism of the compounds.

Keywords: Azoquinoline dye, Azo-hydrazone tautomerism, Solvatochromism, Multi-parameter polarity scale.

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The Study of removal amoxicillin solution from wastewater Pharmaceutical industry by Graphene functionalized carboxylate groups: Langmuir linear forms

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Abstract:

In this research, Amoxicillin from aqueous solutions obtained wastewater Pharmaceutical industry experiment was carried out and then the produced and was used to investigated the adsorption behavior of Amoxicillin from aqueous solutions through UV–Vis spectroscopy at 228 nm as maximum wavelength. The changes of parameters such as contact time, pH, Amoxicillin initial concentration and temperature were tested and investigated by several adsorption experiments. The equilibrium adsorption data were described as well and fitted better by the four linear Langmuir models adsorption isotherm at all studied temperatures and pHs. Moreover, surface structural change was studied for the presence of Amoxicillin and Graphene Oxide (GO) before the experiment by FT-IR spectroscopy. The maximum adsorption capacity of Amoxicillin adsorbed by GO was 50 mg/g calculated by the Langmuir (four type) model at 333 K and pH = 7

Surface was studied by Scanning Electron Microscopy (SEM).acquired during the continuous process of sample heating in the SEM chamber, is shown Figure 1

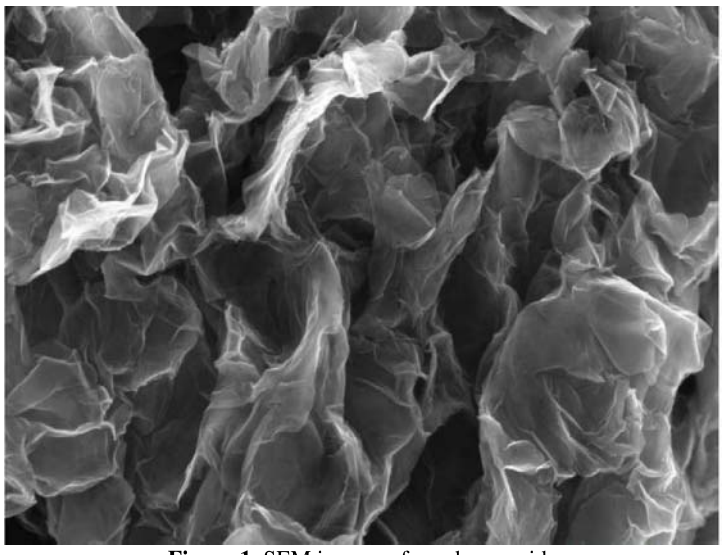

Figure 1. SEM images of graphene oxide

Keywords: Removal Amoxicillin, GO, Langmuir form, FT-IR, Adsorption

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Multiresponse optimization of a turbine oil formulation by mixture design and response surface methods

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Abstract:

The quality and characteristic of a lubricant play a vital role in power plant industry. To achieve optimal performance characteristics, evaluating and monitoring of several integral parameters of steam turbine oils is very important.[1–2] The viscosity indexes (VI), flash point (FP), pour point (PP), and demulsibility are some of these important parameters. At the present work, an extreme vertices mixture design and multiple response optimizations through a desirability function (D) were applied for the first time to formulate and optimize steam turbine oils.[3–7]

We used Design–Expert 7 for all calculations and treatments of data and multiple regression analysis for developing mathemathical models.[4,5] The best fittiting mathematical model was selected based on the evaluation of several statistical parameters including CV, R^2, adjusted R^2, predicted R^2, PRESS, demonstrated by design expert software 7. According to this information linear model was chosen.[6]

According to ISO grade 46 for turbine oils the PP and demulsibility were minimized and FP and VI were maximized.[3] The experimental design were carried out, by using solvent neutral-500 (SN-500), SN-100, polyisobutene (PIB) and antioxidant (BHT). The finalized optimum formulation consist of 22% SN-500, 74% SN-100, 3.0% PIB and 0.4% BHT. Validation was performed in triplicate and display that there were no difference between the estimated and experimental values.

Keywords: Turbine oil, Polyisobutene, Butyl hydroxytoluene, Solvent neutral, Mixture design, Response surface methodology

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Effect of CN functional group on the molecular and electronic properties of BC2N zigzag nanotube

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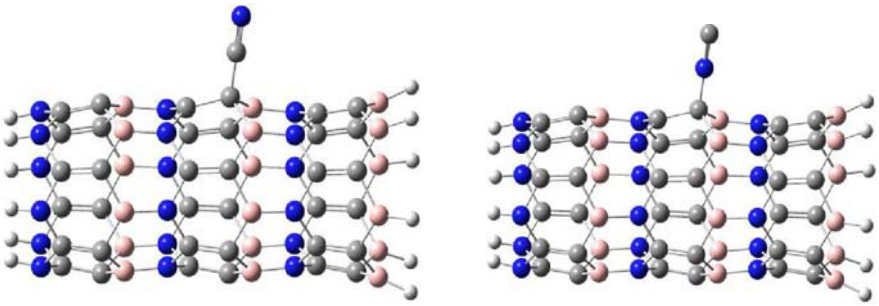
Abstract

The behavior of the CN radical adsorbed on the external surface of BC2N nanotube was studied by using density functional calculations. Geometry optimizations were carried out at the B3LYP/6-31G* level of theory using the Gaussian 03 suite of programs. The energy gap between the highest occupied molecular orbital (HOMO) in gas were calculated. Results indicate that the functionalization results significant changes in their electronic properties. It is predicted that the conductivity of the nanotube increases upon adsorption of radical on the tube. The results obtained by natural bond orbital (NBO) analysis have shown that the charge transfer occurs from functional group to nanotube.

We selected a (6,5) BC2NNT consisted of 18 B, 18 N and 36 C in which the end atoms have been saturated with hydrogen atoms to reduce the boundary effects. Geometry optimizations, energy calculations and natural bond analysis (NBO) have been performed on BC2NNT and different CN/BC2NNT complexes using B3LYP functional augmented with an empirical dispersion term (B3LYP-D) with 6-31G (d) basis set using the Gaussian 03 suite of programs. The B3LYP has been demonstrated to be a reliable and commonly used functional in the study of different nanostructures. We have defined the adsorption energy in the way as: E_{ad} = E(CN) + E(BC2NNT) – E(CN/BC2NNT) where E(CN/BC2NNT) corresponds to the energy of the BC2NNT, in which CN radical has been adsorbed on the surface, E (BC2NNT) is the energy of the isolated tube, E (CN) is the energy of a single CN molecule.

We have investigated all the possible sites for adsorption of CN group on the sidewall of BC2NNT. A CN radical can approach the nanotube walls from outside (out). For the adsorption of the CN radical(N- down and C-down) on the BC2NNT, we considered four possible sites (the C1, C2, N and B sites on the middle ring of nanotube).

For the BC2NNTs the calculated BE (Table 1) for CN in C-down is a little more than that in N- down. Also, CN radicals prefer to interact with C atom in the tube. It seems that pristine BC2NNTs can be used as a CN storage medium as long as CN is adsorbed on the exterior walls of the BC2NNTs because of the high binding energy. In this study the presence of the CN radical, slightly decreases the energy gap of pristine BC2NNTs and increases their electrical conductance The results obtained by natural bond orbital (NBO) analysis have shown that the charge transfer occurs from functional group to nanotube.[1-5]



Bb Ba

Fig. 1. Some optimized structures of CN-BC2N65ZZ nanoptubes

Table 1.Electronic binding energy (kJ/mol) and equilibrium tuberadica

Structure	E	H-L
Nanotube		3.23
Bb	-2975.84	-1.633
Cb	-2956.32	-2.81
Ab	-2944.7	-2.80
Aa	-2910.86	-2.82
Ca	-2874.24	-2.19
Ba	-2864.9	-2.84
Db	-2756.7	-2.85

Keywords: Functionalized Nanotube, Electronic Properties, Adsorption, NBO

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گروه تولیدی صامت تک خزر با هدف ایرانی کردن دانش تولید اسانس‌های طبیعی خوراکی و فرهنگ سازی استفاده از محصولات بهداشتی یکبار مصرف در سال ۱۳۸۲ در شهر صنعتی رشت پایه گذاری شد و در سال ۱۳۸۴ فعالیت خود را در زمینه تولید ساشه های بهداشتی یکبار مصرف با پروانه ساخت از وزارت بهداشت ، گواهینامه استاندارد خود اظهاری و همچنین گواهینامه سیستم مدیریت کیفیت **ISO 9001:2008** از **DQS** آلمان آغاز نمود . هدف گروه تولیدی صامت تک خزر تولید محصولاتی با کیفیت بالا با به روز کردن مداوم سیستم تولید و ماشین آلات می‌باشد که این مهم ازطریق به خدمت گرفتن تکنیک‌های روز، ما را قادر ساخته تا کیفیت محصولات خود را تضمین نماییم و رضایت مشتریان خود را با در نظر گرفتن ویژگی‌ها و نیازمندی آنها تامین نماییم.

هم اکنون گروه تولیدی صامت تک خزر که محصولات آن با نام آشنای **نیوساد** تولید می شود درتمامی استان ها نماینده و عامل توزیع فعال دارد.شایان ذکر است نیوساد یک کلمه فارسی به معنی "بی زوال و فنا ناپذیر" می‌باشد.

واحد **R&D** گروه تولیدی صامت تک خزر با توجه به امکانات گسترده تحقیقاتی و فنی خود در زمینه تولید محصولات آرایشی و بهداشتی با پایه طبیعی و عدم استفاده از نگهدارنده های پارابنی در خدمت مصرف کنندگان محترم می باشد.

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