



Theoretical investigation of energetic performance and impact sensitivities of nitro and trinitromethyl substituted ozonides of ethylene and cyclopentene

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ABSTRACT

A series of novel energetic compounds were designed by introducing groups such as $-\text{NO}_2$, and $-\text{C}(\text{NO}_2)_3$ to the ethylene ozonide (trioxolane) and cyclopentene ozonide (6,7,8-trioxabicyclo[3,2,1]octane) skeletons and their detonation properties and impact sensitivity were investigated using DFT - B3LYP method with aug-cc-pVDZ as basis set. We could design compounds with densities $>2 \text{ g cm}^{-3}$. Most of the compounds exhibit high heat of formation and excellent detonation properties, predominant over traditional energetic compounds. The impact sensitivities of many compounds satisfy criterion of energetic compounds. The compounds containing trinitromethyl (TNM) groups are found to have excellent detonation performance. Also, in trioxabicyclo[3,2,1]octane derivatives, compounds containing TNM group on one of the carbon atoms which was unsaturated in the parent cyclopentene were found to be more stable, addition of NO_2 group on the other carbon enhances the properties as well.

1. Introduction

For the last few years scientists have been in continuous search to discover new high energy density materials (HEDMs) having better thermal stability, insensitivity, superior performance, also for economically and eco-friendly syntheses in order to meet the future demand of civil and military requirements [1,2]. Nitro compounds are a class of high energy density materials and are widely used as explosives [3,4]. Heterocyclic nitrogen compounds such as 1,3,4,6-tetranitroglycouril (TNGU) [5], hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) [6,7] and 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) [8,9] are well known due to their high positive heat of formations and excellent detonation properties. Fused heterocyclic compounds are also known due to their energetic performances [10–13]. Extensive studies have been going on the energetic nature of derivatives of nitrogen heterocyclic compounds such as pyridine [14], azete [15] and aziridine based compounds [16]. Nitrogen rich heterocyclic compounds, such as, azole and tetrazine [17,18] based energetic materials are often used as explosives due to the reduced sensitivity and good thermal stabilities of the resulting compounds [19,20].

In 1982, Kuczkowski isolated the ethylene ozonide (1,2,4-trioxolane)

and described the formation and mechanism [21]. Also, in 1983, Borseth et al. synthesized cyclopentene ozonide (6,7,8-trioxabicyclo[3,2,1]octane) and successfully assigned its structure [22]. In this paper we have designed and theoretically studied the detonation properties and impact sensitivity of a series of novel nitro group and/or trinitromethyl (TNM) substituted ozonide derivatives of simple unsaturated molecules such as ethylene and cyclopentene. Cyclic peroxides are strained heterocyclic compounds containing relatively weak O—O bonds. Generally peroxide based explosives are extremely sensitive to shock, heat, and friction and have no commercial or military applications [23,24]. Common peroxide based primary explosives like triacetone triperoxide (TATP) and diacetone diperoxide (DADP) are mainly used in improvised explosive devices (IED). These compounds lack nitro groups, metallic elements and aromaticity compared to other common explosives. Some sterically hindered peroxides are however reported to be more stable [25–28]. Here we selected the stable ozonides and a series of compounds were designed by systematic incorporation of potential groups such as nitro group and TNM group. This will help the compounds to become energetic.

Introduction of nitro group to a parent heterocyclic compound is a better way to increase the performance of high energy molecules.

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Theoretical studies of azete based high energy density materials with trinitromethane functional group

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ABSTRACT

A series of azete based high energy density molecules, with trinitromethane functional group, were designed and theoretically investigated. The structure optimization, frequency calculations and bond dissociation energies of these compounds were studied using the Gaussian 09 set of programs by the DFT - B3LYP functional (aug-cc-pVDZ). The calculated values of the heat of formation and detonation properties, of these sixty five designed molecules, showed that many of them have excellent detonation properties, with a very high detonation velocity and detonation pressure, >10 km/s and 48 GPa respectively. Most of them were proved to be promising candidates as HEDMs, having thermal stability and impact sensitivity, comparable to traditional energetic molecules, RDX and HMX. From these systematic studies carried out, seventeen molecules were screened out to be the best potential candidates.

1. Introduction

In recent years, there had been a rapid development in the area of high energy density materials (HEDMs) from the efforts of both synthetic and theoretical researches. With the rapid development of computer technology, the theoretical study of HEDMs is of much useful for screening the candidates, not only for avoiding the dangers in the explosion process but also from unwanted reactions [1–4]. Although researches in the field of HEDMs has grown to energetic salts and cocrystals, development of new covalent compounds as HEDMs, is still a developing area [5,6]. The newly designed HEDMs should possess high density, high detonation performance, including high detonation velocity and pressure, good thermal and mechanical stability, and low sensitivity [7]. However, it is difficult to design such a compound since these include contradicting properties [8,9]. Generally speaking, greater the explosive performance, greater the sensitivity of the material [10,11].

The introduction of energetic functional groups such as nitro, nitroso, nitramino, azide groups, etc., into heterocyclic compounds, is one of the best way to design new HEDMs [12,13]. Among these trinitromethyl (TNM) functional group, due to its high nitrogen and oxygen content, positive oxygen balance and high energy has attracted considerable attention [14–17]. The TNM derivatives of three membered

heterocyclic ring compounds are found to be highly energetic [18]. Another tactic for the design of HEDMs includes, utilizing ring or cage compounds, which can take advantage of the extra strain energy released during the ring opening when the decomposition takes place [2,19].

Research in the area of four-membered heterocyclic compounds as HEDMs has not been investigated that much. The most interesting one is 1,3,3-trinitroazetidine (TNAZ), a possible replacement for TNT [20]. The theoretical study of N_4H_4 isomers by Lai-Cai Li showed that they possesses good detonation characteristics [21]. Thus we have selected four-membered heterocyclic compound, namely, azete, as the parent skeleton and have substituted the hydrogen atoms with the energetic nitro groups and trinitromethyl (TNM) groups. Herein, we have designed sixty five such compounds, and a detailed theoretical study of the performance and sensitivity of the compounds were done (scheme 1).

2. Computational methods

Density functional study has been proved to be the one of the best effective and economical tool for the study of energetic materials. First of all, we have performed the geometry optimisation of the designed molecules in the Gaussian 09 set of programs [22] by the DFT - B3LYP

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Detonation properties and impact sensitivities of trinitromethane derivatives of three-membered heterocyclic ring compounds

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ABSTRACT

We have carried out the design and theoretical investigation of a series of trinitromethane derivatives of three-membered heterocyclic ring compounds – aziridine, 1H-azirine, diaziridine, 1H-diazirine, triaziridine, 1H-triazirine, oxaziridine, oxadiaziridine, dioxaziridine, oxirane, and dioxirane – in search for new high energy density materials (HEDM). We have estimated the properties relevant to HEDMs of the proposed molecules using Density Functional Theory (B3LYP/aug-cc-pVDZ). The results show that most of the molecules have a high value of solid-phase heat of formation, crystal density, detonation velocity and pressure with satisfying values for impact sensitivities. We have identified some of these molecules, 1-(trinitromethyl)diaziridine, 2-(trinitromethyl)-1-nitro-1H-azirine, and (2-(trinitromethyl)-3-nitrooxirane) are potential candidates of energetic molecules among the 60 molecules we investigated. As most of them are having a high positive oxygen balance, they can be recommended for use as oxidisers in solid propellants.

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1. Introduction

The design of new high energy density materials (HEDM) with high detonation performance and insensitivity is often a challenging problem [1,2]. Traditional energetic materials such as 2,4,6-trinitrotoluene (TNT), 1,3,5-trinitro-1,3,5-triazinane (RDX), and 1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) derive most of their energies from the oxidation of the carbon backbone [3–5], whereas nitrogen-rich energetic materials derive energy from their high positive heats of formation [6–9]. Polynitro-substituted cage compounds such as hexanitrohexaazaisowurtzitane (CL-20) and octanitrocubane (ONC) release energy upon detonation as a consequence of strain of the cage structure [10]. The design of novel molecules is based on the insights from the traditional materials and by tuning for a high crystal density and chemical energy of detonation.

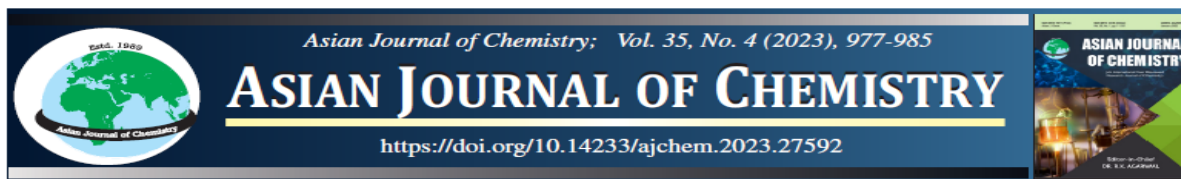
Heterocyclic compounds are of considerable interest as HEDM due to their high density, high positive heat of formation (HOF), better oxygen balance, good thermal stability, and low sensitivity

[11–14]. The strained ring compounds such as ethylene oxide, oxadiaziridine, triazirine, and triaziridine exhibit high performance as they release a large amount of strain energy during ring opening [15–18]. The introduction of explosophoric groups such as O–NO₂, N–NO₂, C–NO₂, –NHNO₂, –N₃, and –C(NO₂)₃ make the compound exhibit superior detonation performances [19–22]. Among these groups, the trinitromethyl functionality possesses both the benefits of high nitrogen and oxygen content, thus found to be an important energetic group [23–26]. Tartakovskii et al. had reported the synthesis of trans-1,2,3-tris(nitramino)cyclopropane (NACP) [18]. The detonation performance studies of a series of nitro-triaziridines showed that the oxygen balance must be considered for designing high-energy compounds [27]. DFT study of a series of ethylene oxide derivatives showed that they have good thermal stabilities [15,28]. Works on the energetic properties of oxadiaziridines showed that they are potential energetic candidates [17,29].

Theoretically examining the molecular structure and properties of a compound allows the selection of powerful and productive HEDM reducing expensive and risky experiments [30–32]. Here we have designed 60 novel derivatives of three-membered ring compounds aziridine, 1H-azirine, diaziridine, 1H-diazirine, triaziridine, 1H-triazirine, oxaziridine, oxadiaziridine, dioxaziridine, oxirane, and dioxirane by introducing trinitromethyl (TNM) and nitro

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3. Publications



Thermal, Mechanical and Swelling Studies of Semi-Interpenetrating Polymer Network Composed of Natural Rubber and Polyacrylamide

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Semi-interpenetrating polymer network (IPN) composed of two polymers, namely natural rubber (NR) and polyacrylamide (PAAm) were prepared by crosslinking with glutaraldehyde. The NR/PAAm semi-IPN films were developed by varying the concentration of crosslinking agents and the polymer blend ratios. The impact of preparation parameters on the mechanical properties was studied. The semi-IPN was characterized by FTIR, DTG, TG and SEM. Swelling studies were done by using toluene as solvent. The kinetics and mechanism of swelling were investigated and the initial rate of swelling, swelling constant, swelling exponent, equilibrium swelling and diffusion coefficient were also determined.

Keywords: Semi-IPN systems, Mechanical properties, Swelling studies, Diffusion coefficient.

INTRODUCTION

A relatively new group of polymeric network systems containing two or more polymers in which at least one of the polymers gets crosslinked in the immediate presence of other are called interpenetrating polymer networks (IPNs) [1,2]. Separation of the network is not possible without breaking the natural bonds. Even though there are no chemical bonds holding these networks together, they are found to be linked in such a way that they will not become separated. Synthesis of IPNs can be performed by blending methods and polymerization processes such as sequential, simultaneous, *etc.* [3-5].

Interpenetrating polymer networks (IPNs) based polymer systems display various characteristics varying from hardened elastomers to high-strength plastics [6]. The final properties of a newly designed IPNs are based on the composition of the polymers under study, the concentration of crosslinking agent used, the physical nature of the constituent polymers, *etc.* [7,8]. IPNs are divided into two categories, semi and full, based on the crosslinking behaviour of the component polymers [9] and can be prepared in different manners. One method is by mixing two simultaneously polymerized and cross-linked monomers

or by dissolving a monomer in a polymer network [10]. Another method for IPNs is by mixing two thermodynamically miscible polymers and crosslinked subsequently. In full IPN, the two polymers form a network of crosslinked structures, even though bonding between the two polymers is negligible [11].

Natural rubber (NR) and polyacrylamide (PAAm) are two familiar polymers and have long been used for many industrial applications, especially as an elastomer for many applications in the engineering field [12]. Its poor thermal stability, easy diffusion of organic solvents and non-compatible with the human body are considered to be its drawbacks [13-15]. Due to these drawbacks, it has been merged with several polymers. For example, chitosan [6,16], cellulose [17], polypropylene [18], polyacrylic acid [19], polyethylene [20] and polystyrene [21]. Polyacrylamides are the water-absorbent polymers forming a soft gel when hydrated [22], since they contain aquaphobic polyethene chief framework and a water loving CONH₂ lateral group. In this work, a semi-IPN composed of natural rubber and polyacrylamide in the presence of glutaraldehyde as cross-linker, through a sequential technique is prepared and its properties were compared with the natural rubber alone. The effect

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Short communication

Cu doped graphitic C₃N₄ for *p*-nitrophenol reduction and sensing applications

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ABSTRACT

A series of Cu doped graphitic carbon nitride (g-C₃N₄) catalysts with different ratios of copper were synthesized by thermal method, using urea and copper sulphate as precursors. XPS (X-ray Photoelectron Spectroscopy) studies indicated that the peak of N1s at 398.9 eV is due to Cu—N bond and a peak at 932.9 eV showed the presence of Cu—N—C bond. Catalytic hydrogenation of *p*-nitrophenol (Para-NP) to *para*-aminophenol (Para-AP) in presence of g-C₃N₄ (gCN) and copper doped g-C₃N₄ (CN-Cu) with sodium borohydride (NaBH₄) was investigated by UV-Visible spectroscopy. The as-synthesized graphitic carbon nitride with 1% copper (CN-1Cu) doped sample exhibits superior catalytic performance and higher stability compared to fine Cu powder in the second cycle. Additionally, electrochemical paracetamol sensing properties of the samples were studied using cyclic voltammetry and chronoamperometry. Consistent with the catalytic performances, CN-1Cu exhibited greater sensitivity towards the detection of paracetamol within the broad range of 38 μM to 3.64 mM and the study was carried out in the physiological pH – 7.4.

1. Introduction

In recent years, graphitic carbon nitride (g-C₃N₄) nanosheets, a special class of 2D materials with layered organic frameworks of carbon and nitrogen have received growing and remarkable attention due to their exceptional physicochemical and thermodynamic properties [1]. Carbon nitride is a non-toxic, metal-free and inexpensive semiconductor material, identical to graphene in its two-dimensional layered morphology with carbon to nitrogen in the ratio (C:N) of 3:4 [2,3]. In comparison to other semiconductors such as ZnO and TiO₂, g-C₃N₄ can be easily synthesized using a variety of methods and has desirable electrical structure and morphology, as well as high thermal stability up to 600 °C.[4] It has gained significant importance in several emerging

applications such as sensors, water splitting, fuel cells, energy storage devices, and transparent conductors due to their unique properties such as greater charge carrier mobility and high mechanical-thermal-chemical stability [3–8].

Owing to their fascinating properties, g-C₃N₄ has been widely being investigated for their catalytic properties by several groups. In one of the recent studies, Gholpour et al. described that mesoporous g-C₃N₄ catalysts can be used for the conversion of alcohols in presence of CO₂ and O₂ or N₂ [9]. Sarkar et al. reported that Cu doped g-C₃N₄ shows excellent electrocatalytic performance towards oxygen reduction reaction in the basic medium [10]. Mohammadi et al. developed copper oxide nanorods decorated with g-C₃N₄ nanosheets for the synthesis of primary amide in water [11]. Covalently bonded sulfamic acid graphitic carbon nitride

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CdS nanosheets as electrode materials for all pseudocapacitive asymmetric supercapacitors

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Abstract. Metal sulphides have recently been explored as a very promising pseudocapacitor electrode, owing to their unique physical, electronic and electrochemical properties. This study reports the synthesis and pseudocapacitor applications of 2D cadmium sulphide (CdS) nanosheets deposited on Ni foam via electrophoretic deposition method. Comprehensive morphological and electrochemical analyses were performed to elucidate the correlation between the structural features of CdS and their charge storage properties. The single electrode characterizations of CdS could exhibit a specific capacitance as high as 1165 F g^{-1} at 2 mV s^{-1} . An asymmetric supercapacitor prototype was also fabricated using the CdS nanosheets with ceria-titania nanotube composite (CeO_2 -TNT) counter electrode. The device could exhibit an energy density as high as 14.58 Wh kg^{-1} at a power density of 1.9 kW kg^{-1} . At the end of 2000 cycles, the device could retain 100% of its initial capacitance.

Keywords. CdS nanosheets; electrophoretic deposition; pseudocapacitance; asymmetric supercapacitor.

1. Introduction

It is of great significance to build up ecofriendly and renewable energy sources and energy storage systems to beat the ever-increasing energy demand and the challenges associated with the use of fossil fuels [1]. Supercapacitors are one of the new generation energy storage systems that offer a very high power density and long cycling life. They are also considered as a green energy storage system, owing to their long cycling life, safe operation, environmental friendliness and capability to work in ample range of temperatures [2,3]. Supercapacitors have found their role in a range of applications like portable electronic devices, backup power supplies, load cranes, forklift, electric utilities and hybrid electric vehicles [4,5]. However, considering to replace or even complement batteries with supercapacitors possess a major challenge; i.e., their lower energy density. Therefore, efforts are under way to improve the energy density of supercapacitor systems by various means.

Generally, supercapacitors can be grouped into three categories based on their energy storage mechanism or cell configuration, i.e., electric double-layer capacitors (EDLCs), pseudocapacitors and hybrid supercapacitors. EDLCs store charge through electrostatic interaction at electrode–electrolyte interface. In EDLC's energy is stored

non-Faradaically, and there is no charge transfer and redox reaction [6]. Unlike EDLC's, pseudocapacitors store charge through Faradaic process, which involves fast and reversible redox reactions between the electrode materials and electrolyte [7]. The specific capacitance and energy density of pseudocapacitors are generally found to be higher than EDLC's, as more charge can be stored both on surface and bulk of the electrode materials by electrochemical process and being a Faradaic system. Hybrid supercapacitors utilizes both the properties of EDLC and pseudocapacitors, in order to achieve higher power and energy density. On the basis of electrochemical configuration of supercapacitor device, supercapacitors can be also classified as symmetric and asymmetric. Symmetric supercapacitors are fabricated using identical electrodes, whereas asymmetric supercapacitors (ASC) are made of two different electrodes [8]. As we have two different electrodes in ASC, during charge–discharge process, we can take the benefit of two different potential windows of the electrodes in order to increase operating voltage of the full device [9]. Thus, an increase in operating voltage results in an increase in both energy density and capacitance value. Considering these facts, it would be beneficial to design an asymmetric pseudocapacitor system with appropriate choice of positive and negative electrodes to improve the storage and power



Visible light photoactivity of 2D nanocomposites of CdS-TiO₂ and CdS-TiO₂-rGO

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ABSTRACT

The CdS-TiO₂-rGO composites of various molar ratios were prepared through a modified solvothermal/hydrothermal process. X-ray diffraction and scanning electron microscope were used for the morphological and structural characterization of the material. The sheet like morphology of the titania and CdS were clearly evident from the scanning electron microscope image of the samples. The composite 2CdS:1TiO₂:rGO(1%) shows highest activity with rate constant 0.00258 min⁻¹. Ultrathin two dimensional sheets-like structure, electrostatic interaction, and presence of rGO (reduced graphene oxide) as supporting matrix are attributed to the highest photocatalytic performance of this composite.

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1. Introduction

Photocatalysis is one of the widely used technologies or promising tool for the environmental cleanup process. A number of carbon based materials and semiconductors are used for photocatalysis. The physical and chemical properties of nanostructures are influenced by the size and shape of materials [1]. Two dimensional semiconductors, have a broad space in research due to their high charge transport property compared to other nanostructures since charge carriers are constricted by finite thickness, they can move through plane freely [2]. Additionally, ultrathin two dimensional nanomaterials have extra ordinary electronic, optical and mechanical properties [3]. Atomically extra ordinary properties of ultrathin two dimensional nanosheets are due to its large specific surface area and strong quantum confinement of the electrons [4]. Moreover exposed crystal facets are the reason for its best catalytic performance [5]. Cadmium sulfide (CdS) is an important semiconductor with a narrow bandgap (2.4 eV) and it has a number of applications in optoelectronic field as in solar cell, light emitting diodes and optical sensors [6,7]. Because of this optimal band gap in the visible region, we can effectively utilize this material for visible light photocatalytic and solar cell applications. The applications of CdS are restricted due to its lesser stabil-

ity and fast recombination of charge carriers. In order to overcome these barriers, different approaches are adopted such as making heterojunctions with organic or inorganic semiconductors, i.e. Z-scheme photo catalytic systems, using co-catalysts [8].

Several attempts are devoted by researchers to construct heterojunction such as graphene or carbon/TiO₂, metal oxide or sulfides/TiO₂ etc. Titanium dioxide (TiO₂) is an important photocatalyst because of its attractive properties like high activity, non-toxicity and low cost. So it is used in purification of air, waste water, production of hydrogen energy, solar cell and photoelectrochemical devices [9]. Preparation of composites with TiO₂ can increase the photo catalytic activity of TiO₂ photocatalyst by extending the photoresponse to visible light and increasing its charge separation of the system. Scientific community has been keen to find out new methods to synthesize TiO₂ based heterojunction composites that are good visible light driven photocatalysts [10].

Another method used to increase the photo catalytic activity is three component Z-scheme method. Three component system has highest photo catalytic activity compared to activities of single or two component system [9]. Electron mediator like graphene is added in Z scheme to promote the transfer of electron between two semiconductor in CdS-TiO₂ system [11]. Longer life time of electron-hole pairs, fast interfacial charge transfer rate and larger surface area are the attractions of three component Z-scheme method [12]. Graphene is a good mediator due to its best trans-

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Growth and characterisation of 5-nitro-2-furaldehyde diacetate single crystals

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Abstract

The 5-nitro-2-furaldehyde diacetate (NFD) single crystals were grown by slow evaporation solution growth technique. By single crystal XRD analysis it was found that, NFD single crystal belongs to monoclinic crystal system. Powder XRD spectrum revealed the crystallinity of the sample. Fourier transform infrared red spectral analysis gave idea regarding the vibrations of functional groups. The transparency of the crystal in the visible region is clearly depicted in the UV–Vis spectrum. Thermo gravimetric/differential scanning calorimetric analysis showed the thermal stability and Vicker's microhardness test showed the mechanical stability of the crystal. From the scanning electron microscopic images, the crystal morphology was analysed. By Kurtz–Perry powder technique, the second harmonic generation efficiency of the NFD crystal is obtained as 15 times greater than that of standard potassium dihydrogen phosphate (KDP) and the laser damage threshold value of the crystal is 4.2 GW/cm², which implies that the sample has got better laser damage withstanding capacity. The studies revealed that, the title compound is a potential candidate for opto-electronic applications.

1 Introduction

Organic nonlinear optical materials with larger optical susceptibility, capability to withstand laser damage, ultrafast response etc., captured constant attention of the researchers because of their wide range of application in electro-optic modulation, optical switching, optical parametric oscillation, high speed information processing and optical data storage [1–4]. Scientists have been working in this area for the last few decades, in search of photonic materials with notable nonlinear response. In addition to this, wider transparency range, higher laser damage threshold, lower absorption cutoff etc. are some other requirements for better NLO response. The presence of extended π bond system attached to the aromatic groups with strong donor and acceptor

groups causes delocalization of electrons [5]. The modern world urges highly capable gadgets. The NLO materials with enhanced second harmonic generation (SHG) efficiency is an inevitable component of such devices. Hence the demand for the synthesis and growth of new potential NLO materials is increasing day by day.

It was reported that certain aromatic heterocyclic compounds with delocalized π electrons are exhibiting good second order nonlinearity [5–8]. In the present work, single crystals of an aromatic heterocyclic organic compound 5-nitro-2-furaldehyde diacetate (NFD) were grown by conventional method with ethanol as the solvent. For the better understanding of the structure and properties of the crystal single crystal XRD, powder XRD, UV–Vis, FTIR, thermal analysis, microhardness, SEM, laser damage threshold and SHG efficiency were studied and discussed.

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2 Materials and methods

2.1 Crystal growth

The powder NFD (AR grade) was dissolved in ethanol to grow NFD single crystals and stirred continuously for 4 h at room temperature to ensure homogeneity of the solution. In order to remove impurities the solution was filtered using

COMPARITIVE CYTOTOXIC STUDIES OF 2-[4-(2-METHYL PROPYL) PHENYL]PROPANOIC ACID AND ITS 1,2,4- TRIZOLE DERIVATIVE ON HEPG2 CELL LINE

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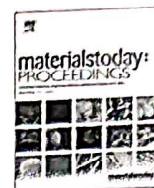
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Abstract: Non-steroidal anti-inflammatory drugs (NSAIDs) are used in the treatment of pain, inflammation, osteoarthritis and rheumatoid arthritis. 2-[4-(2-methyl propyl)phenyl]propanoic acid belonging to NSAIDs. Prolonged use of NSAIDs tends to cause gastrointestinal complications. The use of prodrugs to temporarily mask the acidic group of NSAIDs has been postulated as an approach to decrease gastrointestinal toxicity of these drugs. The 1, 2, 4-triazole is used for designing potential bioactive agents. Derivatives of this structure was prepared by reacting 2-[4-(2-methyl propyl)phenyl]propanoic acid and thiocarbonylhydrazide. The synthesized triazole and the parent compound were then subjected to cytotoxic studies on HepG2 cell line and comparative studies were done.

Keywords: 1,2,4-Triazole, Ibuprofen, NSAIDs, Prodrug, One-pot method.

1. INTRODUCTION

Non-steroidal anti-inflammatory drugs (NSAIDs) such as ibuprofen are widely used in the treatment of pain and inflammation, including osteoarthritis and rheumatoid arthritis [1-3]. Ibuprofen, (2-[4-(2-methyl propyl) phenyl] propanoic acid) is a versatile drug belonging to Non-steroidal anti-inflammatory drugs (NSAIDs) was developed during the 1950s and 1960s as a super aspirin for the treatment of rheumatoid arthritis, to relieve moderate pain, inflammation and fever. Prostaglandins (PGs) are well known to be the mediators of inflammation, pain and swelling. They are produced by the action of cyclooxygenase (COX) enzyme on arachidonic acid. Metabolites of the COX pathway are widely accepted as mediators of the inflammatory response. COX is known to be the principal target of non-steroidal anti-inflammatory drugs (NSAIDs). NSAIDs block the formation of PGs and have analgesic, antipyretic and anti-inflammatory activities [4]. In the early 1990s, it was discovered that the COX enzyme exists as two isoforms, one constitutive (COX-1) and the other inducible (COX-2). COX-1 is constitutively expressed and provides cytoprotection in the gastrointestinal (GI) tract while COX-2 is inducible and mediates inflammation [5-7]. The traditional NSAIDs show greater selectivity for COX-1 than COX-2 [8]. In fact, prolonged use of NSAIDs like ibuprofen has been associated with gastrointestinal complications ranging from stomach irritation to life-threatening GI ulceration bleeding and nephrotoxicity [9,10]. Therefore the development of new NSAIDs without these side effects has long been awaited. Selective COX-2 inhibitors with better safety profile have been marketed as a new generation of NSAIDs [11]. Thus there remains a compelling need for effective NSAIDs with an improved safety profile. Chronic use of NSAIDs, including ibuprofen, may elicit appreciable GI toxicity; [12] therefore, synthetic approaches based upon NSAIDs chemical modification have been undertaken with the aim of improving the NSAID safety profile. The GI damage from NSAIDs is generally attributed to two factors, local irritation by the carboxylic acid moiety, common to most NSAIDs (topical effect) and decreased tissue prostaglandin production, which undermines the physiological role of cytoprotective prostaglandins in maintaining the GI health and homeo-stasis. [13] It has been reported that the derivatization of the carboxyl function of representative NSAIDs, resulted in an increased anti-inflammatory activity with reduced ulcerogenic effect [14].



Fabrication of PPSU/PANI hollow fiber membranes for humic acid removal

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ABSTRACT

Membrane based separation has proved its efficiency over other traditional techniques of water purification. Hollow fiber (HF) membranes are more ideal compared to other types of membranes due to their high surface area, enhanced mechanical property and easy handling. Significant research had been done in this area, still the abundant scope of membrane technology has motivated many scientists to further explore the field. The current work is an attempt to study the efficiency of nanomaterials in polymeric membranes. This paper is focused on incorporating polyaniline (PANI) based nanocomposites into the polymer membranes and to study the properties and performance of the prepared nanocomposite membranes. Polyphenylsulfone (PPSU) and polyvinylpyrrolidone (PVP) are the main polymer and pore forming agent used in this study respectively. The dope solution was prepared by blending PPSU and PVP with PANI in different compositions. New PPSU composite HF membranes were fabricated using wet-jet phase inversion technique. The properties and performance of the membranes were analyzed by cross sectional morphology, water uptake capacity, permeation properties and antifouling ability. The self-cleaning capacity of the membranes was determined by evaluating the flux recovery ratio. The water purification efficiency of the membranes was evaluated in terms of humic acid rejection studies. Polyphenylsulfone containing 0.5 wt% of polyaniline exhibited maximum rejection of 99% for humic acid.

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1. Introduction

Pollution and shortage of potable water across the globe, along with rising population and strict standards of drinking water or waste water discharge, made the membrane filtration as an ideal alternative in future water treatment processes [1]. A membrane is a selective barrier between two phases, separates all particles bigger than its smallest pore size. The smaller compounds may also be rejected by charge repulsion if they have negatively charged groups on it and the membrane is negatively charged. Hence, the removal of particles by membranes increases with decreasing the pore size of the membranes and also with increasing the membrane surface charge density [2]. The efficiency of the membrane filtration increases with increase of membrane surface area per unit of volume of the container. Hollow fiber (HF) membranes

are having high permeability due to its large surface area. So, geometry of hollow fibers is more effective for a separation purpose than any other forms. Moreover, hollow fibers are self supporting and not require any costly support systems [3]. HF membranes can easily be prepared from any spinnable material.

Synthetic membranes face common problems such as high hydrophobicity, fouling, low fluxes and low mechanical strength. The main shortcoming of membrane techniques is their high operational cost because of the fouling nature of membranes. Fouling is caused by the deposition of solute particles or any macromolecules on the membrane surface or inside the pores [4]. Fouling reduces the membrane flux and its performance. Fouling is a serious threat to the wide spread use of membrane filtration technology. Fouling depends on various factors which includes composition of feed solution (concentration of components and pH), membrane properties (hydrophobicity, roughness, pore size, pore size distribution, porosity) and operating conditions (temperature, trans-membrane pressure and cross-flow velocity) [5]. Cross-flow method can be

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