

Structural, thermal, linear and nonlinear optical and cytotoxicity studies of a novel organic stilbazolium salt: 4-[2-(4-hydroxyphenyl)ethenyl]-1-methylpyridinium 4-styrenesulfonate



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ABSTRACT

Organic non-linear single crystals of 4-[2-(4-hydroxyphenyl)ethenyl]-1-methylpyridinium 4-styrenesulfonate (HMSS) are grown by means of slow solvent evaporation growth process. Stoichiometric ratio of the elements existing in the compound is identified by elemental analysis. Single crystal X-ray diffraction discloses that the developed crystal being included in to P2₁/n space group with monoclinic crystal system. In addition, an analysis of crystal structure and Hirshfeld surface are used to expose the intermolecular interaction and hydrogen bonds. Quantum chemical calculations performed using the density functional theory (DFT) at DFT/B3LYP/6-311+G(d,p) level of the compound provides further insight on the properties in particular molecular electrostatic potential, natural bonding orbital analysis (NBO), Mulliken and NPA charges, static dipole moment, polarizability, first order hyperpolarizability and thermodynamic functions. The frequencies (vibrational) of the compound HMSS are recognized using FT-IR and FT-Raman analysis and compared with the calculated data. Thermal properties of HMSS are accomplished via the way of TG and DSC analyses. Further, antiproliferative behavior of the obtained compound is assayed against human breast adenocarcinoma cells MCF 7 and normal Vero cells (monkey's kidney cells).

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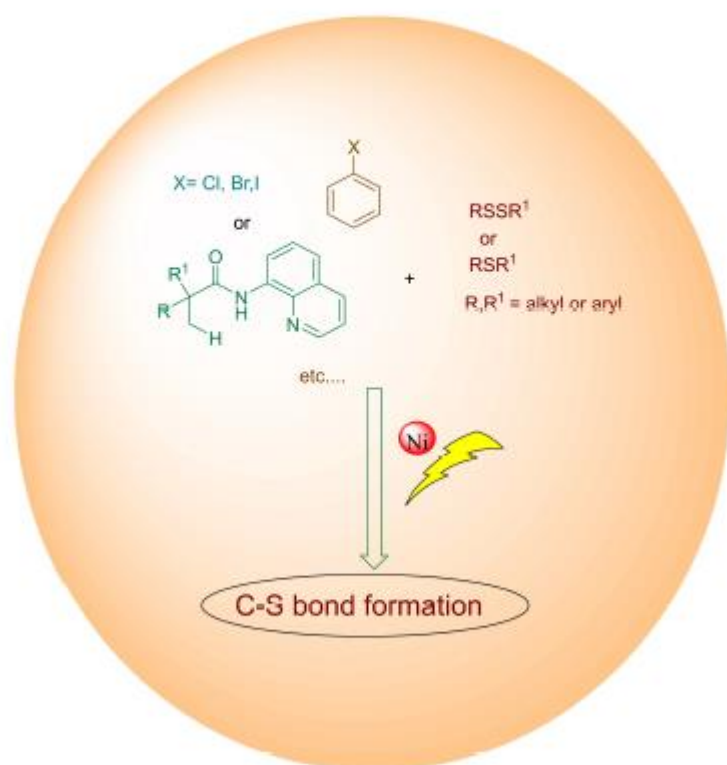
1. Introduction

There is a predominant hopeful concern in organic non-linear optical (NLO) materials compared to inorganics in the field of optoelectronic and bio photonics [1–4]. The organic π -conjugated D-A material with pyridinium units has been receiving

with strong D- π -A intermolecular interaction abides as the origin of the NLO properties. The optical NLO efficiency of organic salts are depended upon strong Coulombic interactions among the π -conjugated chromophore with appropriate electron donor and acceptor groups at the end [9–11]. The styrylpyridinium derivatives are considered to be good conjugated π -systems, and they have been put to practical use for their large NLO effi-

Recent Trends in Nickel-Catalyzed C–S Bond Formation

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Current developments in the synthesis of 4-chromanone-derived compounds

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Abstract:

The chroman-4-one framework is a significant structural entity that belongs to the class of oxygen-containing heterocycles. It acts as a major building block in a large class of medicinal compounds, and synthetic compounds exhibit a broad variety of remarkable biological and pharmaceutical actions. Several studies have been taking place to improve the methodologies of 4-chromanone-derived compounds. This review focuses the major synthetic methods of preparation reported on chroman-4-one derivatives from 2016-2021.

Keywords: chroman-4-one derivatives, cascade radical cyclization, hydroacylations, 2, 3-dihydro-1-benzopyran-4-one, phytochemical.

1. Introduction

Phytochemicals are non-nutritive plant chemical, includes chromones,¹ coumarins,² chalcones,³ carotenoids⁴ or flavonoids⁵ showed great biological significance in preventing diseases in human. 4-chromanone-derived compounds (2,3-dihydro-1-benzopyran-4-one) and their research are of immense significance in the area of pharmaceutical chemistry, which plays an important building block in designing drugs.^{1,6} It exhibited broad range of biological and pharmaceutical activities such as antibiotic,⁷ antiparasitic,⁸ anticancer,^{9,10} anti-HIV¹¹ and SIRT2 inhibitors.¹² Chroman-4-one displayed large structural varieties directed to

various biologically important, natural compounds like sakuranetin,¹⁸ Naringin,¹⁹ Eriodictyol,²⁰ Hesperetin²¹ and Sterubin²². Phytoestrogens isoflavones²³ like Genistein,²⁴ Daidzein,²⁵ Glycitein,²⁶ Biochanin A,²⁷ Formononetin²⁸ have significant role in medicinal field, regarded as chemoprotective and hence widely used in cancer treatment, menopausal symptoms, and osteoporosis. Many methods have been established for the preparation of those structural motifs in the previous years.^{29,30} Though, some classical approaches have drawbacks like multi-step procedure, harsh reaction settings, less substrate scope etc. So, still many research works are on-going for introducing more efficient and atom-economical methods to construct this privileged scaffold under mild and environmentally benign conditions. This review focuses on the novel synthetic approaches of chroman-4-one derivatives and covers literature from 2016 to 2021, since the topic has been reviewed in 2015 by Emami and Ghanbarimasir.²⁹ For effortlessness and simplicity, the topic is grouped on the basis of methods of synthesis involved.


2. Synthesis of chroman-4-one derivatives

2.1. Synthesis of chroman-4-one derivatives through cascade radical cyclization

The methods of organic synthesis have progressed to advance promptly. In last few decades, great efforts have been focussed on organic synthesis includes cross coupling reactions,³¹⁻³⁶ functional group interconversions(FGI)^{37,38} and Cascade radical cyclization reactions³⁹⁻⁴¹ which offer a valuable synthetic tool in organic synthesis. The prominent advantages of radical cascade reactions such as high efficiency, environmentally benign as well as economical protocol and great reduction of time duration to complete the work. Recently, in 2020, a Xiong *et al.*⁴² reviewed 3-substituted chroman-4-ones by radical reaction. Currently, chroman-4-one derivatives are synthesised through the cascade reactions with *o*-(allyloxy) arylaldehydes as initial material through radical process have gained considerable attention.



Recent developments of supported Palladium nanocatalyst and magnetically separable supported Palladium nanocatalysts for Heck cross-coupling reactions

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Abstract Transition metal nanoparticles (NPs) have fascinated tremendous interest nowadays, especially in a large variety of carbon–carbon bond-forming reactions due to their high surface area-to-volume ratio and reactive morphologies. This review focuses on the developments in supported palladium nanoparticles and magnetically separable supported palladium nanoparticle-catalyzed Mizoroki–Heck coupling from 2018 to May 2021.

Keywords Mizoroki–Heck coupling · Supported palladium nanocatalyst · Magnetic palladium nanocatalyst · Synthesis

Introduction

with group 8–10 transition metal catalysts, remarkably palladium complexes, is the way of selection for a broad range of C–C (Varun et al. 2017; Kanchana et al. 2020a, b; Jose et al. 2020a; Diana et al. 2020) C–Se (Jose et al. 2020b), C–N (Hosseinian et al. 2018), C–P (Kanchana et al. 2021), C–S (Hosseinian et al. 2019) or C–M bond-forming methods. Mizoroki–Heck cross-coupling is transition metal-catalyzed coupling between aryl halides or vinyl halides with an activated alkene, in the presence of a base resulting in substituted alkene through a new C(sp²)–C(sp²) bond formation (Christoffel and Ward 2018). Richard F. Heck, Ei-ichi Negishi and Akira Suzuki won the Nobel prize in chemistry in 2010 for their studies ‘for palladium-catalyzed cross-couplings in organic synthesis’ (Astruc 2010).

Metal nanoparticles are highly effective catalysts

Mahatma Gandhi and the Harmony of Music

Teresa Joseph
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ABSTRACT

Mahatma Gandhi had actively engaged with music in various ways throughout his life. He had a rather nuanced approach to music, art and aesthetics which can be seen as part of his larger philosophy of life. Drawing from his speeches, writings and interviews, this article discusses Gandhi's engagement with music. It unveils Gandhi's perspectives on art and music as well as music and religion, and his notion of the power of music to transcend sectarian boundaries. It also analyses Gandhi's social practice of music including his interventions in the conflicts relating to music and religion, and the question of democratising music as against its then existing exclusionary nature. The paper provides yet another pathway to understand Gandhi's life and thought, particularly with regard to universal fraternity and religious pluralism.

Key words: Gandhi, music, art for art's sake, music and religion, universal harmony

Introduction

MAHATMA GANDHI CAN be viewed and understood from diverse perspectives and vantage points and through different lenses. Gandhi's engagement with music is one such lens through which one



Ringing non-Gaussianity from inflation with a step in the second derivative of the potential

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Abstract. Inflationary model driven by a scalar field whose potential has a step in the second derivative with respect to the field is considered. For the best-fit potential parameter values, the 3-point function and the non-Gaussianity associated with the featured model is calculated. We study the shape and scale dependence of the 3-point function. The distinctive feature of this model is its characteristic ringing behaviour of f_{NL} . We can see that the oscillations in f_{NL} in this model last for a much longer range of k values, than the previously studied models. In that sense, this model is potentially distinguishable from models with other features in the potential.

Keywords. Inflation; 3-point function; non-Gaussianity.

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1. Introduction

In standard slow-roll inflation, the deviation from the Gaussian distribution of the primordial perturbations [1–3] is predicted to be small. It is of the order of the slow-roll parameters [4–7]. This result does not hold if the inflaton undergoes a period of slow-roll violation during its evolution [8–11], as can happen if the inflaton potential has some localised features [12]. The resulting non-Gaussianity [13] then becomes shape and scale-dependent and modes that exit Hubble scale around the time the field crosses the feature can pick up large non-Gaussianities. An inflationary model, where the inflaton potential has a feature in its second deriva-

[20–23], is discussed there. In the present work, we compute the 3-point function of the curvature perturbation and study the shape and scale dependence of the 3-point function.

The paper is organised as follows: in §2 we describe our model and give its background evolution and resulting power spectrum of curvature perturbations. In §3 we compute the 3-point function and the non-Gaussianity from the model and then conclude by summarising the results in §4.

2. The model with a step in the second derivative of

Contextualising Gandhi, the Plague and Public Health in Pandemic Times

Teresa Joseph*

Abstract

The COVID-19 pandemic has served as a wake-up call to revisit questions of public health and well-being the world over, with insights being drawn from various cultures and systems of medicine. Mahatma Gandhi wrote and spoke extensively on health and hygiene, in the firm belief that public awareness lay at the root of addressing the key notion of prevention rather than cure. His experiences during the outbreak of plague in Johannesburg helped crystallise his vision of health – particularly of the need to view it from the perspective of the disadvantaged sections of society. This paper provides an understanding of Gandhi's vision of health and hygiene.