

**List of publications from the thesis**

1. **Gaurang J. Bhatt**, Pradeep T. Deota, Deepak Upadhyay, Prafulla K. Jha, Site-selective unidirectional benzylic  $sp^3$  C-H oxidation of dodecahydrotriphenylene with  $RuCl_3-NaIO_4$ : Formation of benzylic ketones; *RSC Advances*, 34498, 2021; <https://doi.org/10.1039/D1RA06897K>
2. **Gaurang J. Bhatt**, Pradeep T Deota, Narayan N Som and Darshil Shah, Butterflyene: A smooth entry into an aesthetically pleasing Prototype Decacyclic Ring System via Intermolecular Diels–Alder Reaction on a tetrasubstituted olefin; *Organic & Biomolecular Chemistry*, (In revision)
3. **Gaurang J. Bhatt** and Pradeep T. Deota, Exploitation of  $\alpha$ -position of carbonyls to expand the library of Trindane and Dodecahydrotriphenylene carbocycles; (Manuscript is under preparation)

**List of publications not included in the thesis**

1. Bharat Maru, **Gaurang J. Bhatt**, Urvi Lad, Pradeep T. Deota, Sanjeev Kane, U. K. Goutam, Chetan K. Modi,  $Fe@g-C_3N_4$ : An effective photocatalyst for Baeyer-Villiger oxidation under visible light condition; *New Journal of Chemistry*, 2023, 47, 9797-9805, <https://doi.org/10.1039/D3NJ01292A>
  2. Pradeep Deota, Deepak Singh and **Gaurang Bhatt**, A Short and Facile [2+2] Photocycloaddition Protocol Towards construction of Levuglandin Skeleton; *Pharmaceutical Fronts*, 2023 (Accepted, in press, Preprint)
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available on ChemRxiv), <https://doi.org/10.26434/chemrxiv-2023-hq4xp>

3. Pradeep T. Deota, Hemant S. Parmar, Gautam M. Patel, ***Gaurang J. Bhatt***, Impact of Ultraviolet-Absorbing 2-hydroxy-4-quaternaryammoniumalkoxy benzophenone motif on photodegradation of Disulfoton: A case study; *Environmental Science and Pollution Research-Springer*, 2022; <https://doi.org/10.1007/s11356-022-21247-1>
  
  4. Gautam M. Patel, Vraj R. Shah, ***Gaurang J. Bhatt***, Pradeep T. Deota, Humidity nanosensors for smart manufacturing in Nanosensors for Smart Manufacturing, Ed. Sabu Thomas, Tuan Anh Nguyen, Mazaher Ahmadi, Ali Farmani, Ghulam Yasin; *Elsevier*, 555–580 (2021). <https://doi.org/10.1016/B978-0-12-823358-0.00026-5> (*Book Chapter*)
  
  5. Gautam M Patel, ***Gaurang J. Bhatt***, Pradeep T. Deota, Synthesis and characterization of silicon-based hybrid nanoparticles, in Silicon-Based Hybrid Nanoparticles, Ed. Sabu Thomas, Tuan Anh Nguyen, Mazaher Ahmadi, Ghulam Yasin, Nirav Joshi, *Elsevier*, 11-43 (2021). <https://doi.org/10.1016/B978-0-12-824007-6.00006-X> (*Book Chapter*)
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# Site-selective unidirectional benzylic $sp^3$ C–H oxidation of dodecahydrotriphenylene with $RuCl_3-NaIO_4$ : formation of benzylic ketones†‡

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Dodecahydrotriphenylene, a higher homologue of trindane chemoselectively undergoes unidirectional benzylic  $sp^3$  C–H oxidation and the central benzene ring remains intact unlike that in trindane under similar reaction conditions.  $RuO_4$  which generally attacks  $sp^2$  C–H to form oxidative products is found to give benzylic ketones *via*  $sp^3$  C–H oxidation. Density functional theory (DFT) calculations have also been performed to analyse the potential energy, energy barrier and HOMO–LUMO energy gap of the products.

## Introduction

Selective transformation of benzocyclotrimers (BCTs) into their keto derivatives is highly desirable due to the diverse utility of the keto functionality in various synthetic elaborations towards graphene and buckminsterfullerene (Fig. 1). Hence, selective benzylic oxo-functionalization of alkylarenes is an important protocol in organic synthesis.<sup>1</sup> Moreover, benzylic oxidation of alkylarenes provides valuable synthons that can lead to many natural products, agrochemicals and pharmaceuticals.<sup>2</sup>

There are numerous reagents reported in the literature for selective benzylic oxo-functionalization such as  $NaClO/TEMPO/Co(OAc)_2$ , *o*-iodoxybenzoic acid,  $KMnO_4/MnO_2$ , bismuth-picolinic acid, *t*-BuONa, and ascorbic acid.<sup>3</sup> Ruthenium complexes have been commonly employed in various oxidative transformations to furnish a variety of oxo-functionalities.<sup>4–6</sup>

In general, Ru-compounds have been shown to attack alkenes *via*  $sp^2$  C–H activation to form aryl ketones.<sup>7</sup> However,  $RuCl_3-NaIO_4$  has been reported to exhibit poor reactivity during benzylic oxo-functionalization of alkylarenes *via*  $sp^3$  C–H activation.<sup>8a</sup> Hence, complexes of ruthenium have been employed to accomplish effective benzylic  $sp^3$  C–H oxidation of aromatic hydrocarbons to corresponding aromatic ketones.<sup>8b</sup>

Interestingly, the oxidation of tricyclopentabenzene (trindane, **1**) has been shown to yield a highly functionalized tricyclic system **2** (Scheme 1) upon oxidation with ruthenium tetroxide generated *in situ*.<sup>9</sup> It is remarkable to note that the compound **1** undergoes complete cleavage of the central benzene ring.

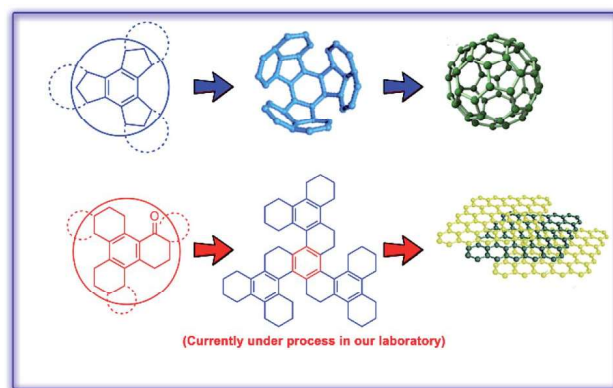
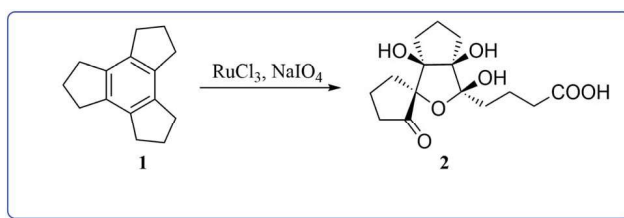


Fig. 1 Benzocyclotrimer precursors towards fullerene and graphene.



Scheme 1 Ru(VIII) mediated oxidation of the benzene ring of trindane **1**.

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† The authors have dedicated this paper to Prof. Vishwakarma Singh on his 70<sup>th</sup> birthday.

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# Fe@g-C<sub>3</sub>N<sub>4</sub>: an effective photocatalyst for Baeyer–Villiger oxidation under visible light condition†

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In this work, we fabricated peculiar and highly cogent iron-doped graphitic carbon nitride (Fe@g-C<sub>3</sub>N<sub>4</sub>) nanocatalysts with varying ratios of g-C<sub>3</sub>N<sub>4</sub> nanosheets to Fe-dopant in 1:1, 1:3, and 1:5, respectively. Numerous physicochemical techniques, including high-resolution transmission electron microscopy (HRTEM), Fourier transform infrared (FTIR), powder X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) were used to validate the as-synthesized catalysts to explain their morphology and chemical structure. In addition, it was revealed that Fe metal ions were well disseminated with no alteration in the layered stacking structures of the g-C<sub>3</sub>N<sub>4</sub> nanosheet and/or might interact with N atoms of the graphitic plane, forming intercalation compounds, thereupon influencing the energy band structure, augmenting visible light absorption, and electron–hole rupture rate. Under visible light (12 W) conditions, Fe@g-C<sub>3</sub>N<sub>4</sub> (1:1) has shown superior performance for selective Baeyer–Villiger oxidation reaction, giving 100% cyclohexanone conversion and an admirable product selectivity of 2-oxepanone, *i.e.*, 99.85%. Besides, the main advantages of the present catalyst include its excellent reusability up to five repeated cycles with no significant loss of activity.

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## 1. Introduction

These days, the advancement of green and potent technological ways to resolve ecological problems is a major point of debate that scientific research has to resolve. Semiconductor-based photocatalysts can realize adequate conversion along with the storage and consumption of solar energy, and run valuable chemical reactions under benign conditions by way of precisely utilizing solar energy.<sup>1</sup> Various traditional semiconductor-based photocatalysts have been reported for environmental restoration so far.<sup>2–4</sup> TiO<sub>2</sub> is the most extensively researched semiconductor-based photocatalyst due to its superior photochemical stability, inherent oxidation aptitude, great hydrophilicity, and innocuous nature.<sup>5,6</sup> However, the downside of TiO<sub>2</sub> is that it is effective only under the conditions of ultraviolet light, utilizing about 4% of sunlight, thus substantially hampering its

practical applications.<sup>7</sup> Thus, emerging new photocatalysts with the advantages of high quantum efficiency, ease of visible light utilization, high strength, and significantly low cost are now in high demand in the field of photocatalysis.<sup>8,9</sup>

In the last few years, the focal point of photocatalytic research has been centered on polymeric semiconductor-based materials, *i.e.*, graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) as a visible light induced photocatalyst owing to its notable semiconductor band structure and exceptional chemical stability. It has been widely used for photocatalytic H<sub>2</sub> and O<sub>2</sub> production, selective photocatalytic organic synthesis, and degradation of organic and/or inorganic pollutants photocatalytically under visible light.<sup>10–15</sup> On the other hand, due to its polymeric nature, some problems still persist in using g-C<sub>3</sub>N<sub>4</sub> as a photocatalyst, such as small specific surface area, crucial photo-induced electron–hole recombination, low quantum yield, and extensive bandgap, which slow down the adequate utilization of sunlight.<sup>16</sup> Despite this, studies have shown that C<sub>3</sub>N<sub>4</sub>'s photogenerated electrons are localized within tri-s-triazine-based building blocks, causing a high recombination rate of electron–hole pairs and preventing photocatalysis.<sup>17</sup> As a result, research has been focusing on ameliorating its photocatalytic activity by manipulating the potential of g-C<sub>3</sub>N<sub>4</sub>'s valence and conducting bands using techniques such as surface modification, metal and non-metal doping, coupling with other

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# Impact of ultraviolet-absorbing 2-hydroxy-4-quaternaryammoniumalkoxy benzophenone motif on photodegradation of disulfoton: a case study

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## Abstract

Pesticide deposits post-treatment and before diffusing inside the plants are exposed to sunlight. Many of them degrade into a variety of photoproducts that may be harmful to living beings through accidental ingestion. The addition of ultraviolet light absorbers to the pesticide formulations is an attractive strategy to prevent photodegradation of the pesticides. Water-soluble quaternary ammonium ultraviolet light absorbers (QAUVAs) were synthesized from 2,4-dihydroxy benzophenones (BP-1) and their structures were confirmed by <sup>1</sup>H NMR, <sup>13</sup>C NMR, UV, and FTIR. A cost-saving approach for the photoprotection of disulfoton insecticide using these QAUVAs is presented. All the four QAUVAs exhibit excellent UV screening effect. The insecticide disulfoton was recovered in much higher amounts (22.27 ~ 25.64% higher than control) when it was irradiated in the presence of QAUVAs in comparison with the amount of recovery of pesticide exposed in absence of them.

**Keywords** Quaternary ammonium salts · Photodegradation · 2,4-dihydroxybenzophenone · Integrated pest management · Disulfoton · Pesticides

## Introduction

Ultraviolet light between wavelengths 280 nm and 400 nm is a major cause of photodegradation of many organic materials such as polymers, agrochemicals, and dyes (Santos et al. 2012; de Lima and Serra 2013; Bojinov et al. 2009; Cordero et al. 2005; Cui et al. 2012; Czajkowski et al. 2006). The addition of ultraviolet absorber (UVA) is an effective way for their protection against damage by UV light as well as for extending their service life (Santa María et al. 2013; Ozáez et al. 2013; Choi and Jang 2011; Cui et al. 2013; Feng et al. 2012; Mahltig et al. 2005;

Zayat et al. 2007). A rapidly occurring excited-state intramolecular proton transfer (ESIPT) via reversible keto-enol tautomerism to release the excitation energy in the form of heat, fluorescence, or phosphorescence is the key feature of these ultraviolet absorbers (Steeley et al. 2014; Dobashi et al. 2007; Kikuchi et al. 2013; Shaath 2010; Maliakal et al. 2002; McGarry et al. 1997; Pickett 2000; Mosquera et al. 1996; Woessner et al. 1984; Klöpffer 1977; Ghigginio et al. 1986; Otterstedt 1973) (Fig. 1).

Some of the well-studied ESIPT fluorophores have been o-hydroxy-substituted aromatic compounds, benzophenone derivatives, benzotriazole derivatives, and benzo-fused heterocycles such as 2-(2'-hydroxyphenyl)benzimidazole (HBI), 2-(2'-hydroxyphenyl)benzoxazole (HBO), and 2-(2'-hydroxyphenyl)benzothiazole (HBT) (Santos et al. 2012; Fent et al. 2014; Liu et al. 2014; Benelhadj et al. 2013; Padalkar et al. 2013b, 2014, 2013a; Cheng et al. 2015; Rodembusch et al. 2005; Majumdar and Zhao 2015) (Fig. 2).

Pesticides and their residues are believed to be degraded in the environment by a variety of natural pathways such as hydrolysis, metabolism by plants and animals, enzymatic processes, and photodegradation (Pehkonen and Zhang 2002). The degraded products and residues of pesticides then can pose potential threat through accidental ingestion by humans and animals along with the agricultural products (Özkara et al.

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# Synthesis and characterization of silicon-based hybrid nanoparticles

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## 2.1 Introduction

One of the most active fields of science today is the area of nanostructured materials such as nanowires, nanorods, nanospheres, and nanobelts (Joshi et al., 2018; Patel, Pillai, Bhatt, & Mohammad, 2020; Patel, Shah, Bhatt, & Deota, 2021; Patel, Vora, & Pillai, 2019; Wu et al., 2020). Specifically, silicon nanoparticles (SiNPs) are a booming and fascinating area of science with major technical implications. SiNPs demonstrate noncytotoxic properties (Park et al., 2009; Sato et al., 2009) and persistent multicolor luminescence of blue light with a reduction of the mean diameter at room temperature (Sato, Kishimoto, & Hirakuri, 2007). The latest interest came nearly a decade after Canham's exciting 1990 discovery (Canham, 1990). SiNPs have a number of significant advantages, such as low toxicity, emissions from a single material across the entire visible spectrum, and silicon's ability to form covalent carbon bonds and thus combine inorganic and organic components at the molecular scale. An additional feature expanding their usage manifold as an extraordinary support material is the possibility of functionalizing both the external and internal pore surfaces with several organic moieties. A number of investigations were conducted to change the surface of SiNPs using alkyl chains in order to make Silicon Nanocrystals (SiNCs) stable in different solutions (Anderson et al., 2012; Báñez-Redín, Joshi, & do Nascimento, 2020; Dasog & Veinot, 2012; Dasog et al., 2013; Joshi et al., 2016; Li & Ruckenstein, 2004; Li, Swihart, & Ruckenstein, 2004; Panthani et al., 2012; Singh et al., 2013). Further practical changes



## CHAPTER 24

# Humidity nanosensors for smart manufacturing

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### 1. Introduction

Currently, temperature can be measured using extremely accurate devices. However, water vapor content of the air, or humidity, is much more complex to measure. Humidity is an important property on our planet, crucial for biological systems as well as our modern automated industries. Therefore sensing, monitoring, and managing humidity under different conditions of temperature and composition are vital to maintaining the necessary ambience. Humidity sensing devices are an area of focus for researchers, primarily because of their significance in numerous functional uses, ranging from households to industries [1–3].

The human eye cannot see the gaseous phase of water, called water vapor. Humidity may be in the form of precipitation, fog, or dew. As the temperature rises, the water vapor saturation increases, and vice versa. The quantity of water vapor suppressed inside a parcel of air can differ considerably. There are three principal measurements of humidity generally employed: absolute, relative, and specific. The total content of water vapor existing in a unit volume of gas is represented in grams of water per cubic centimeter of air, known as absolute humidity. The ratio of amount of water vapor in the air to the maximum amount of water vapor that can be contained in the air at a temperature is known as relative humidity, expressed as a percentage. Thus the air can be said to have 100% relative humidity when it is saturated with water vapor, or 0% if there is no water vapor present in it. Specific humidity, also known as moisture content, is the relation of water vapor mass to the total moist air parcel mass [4].

Moisture sensors measure the content of water vapor in either sterile gas or a fusion of gases. Usually, the humidity is described in terms of dew/frost point, relative humidity and parts per million [5]. Relative humidity expressed in percentage is a relative measurement and is a function of temperature. On the other hand, dew/frost point is a function of pressure and is an absolute measurement of humidity [6]. The water vapor in air or gas converts to liquid form through cooling at a certain temperature, called the dew point. The temperature at which water vapor condenses to solid form, ice, is called the frost