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# Analysing the Chemical, Physical and Biological Properties of Fullerenes as A Therapeutic Agent

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***Abstract-* The unique electrical and structural features of fullerenes and similar carbon-based derivatives make them great candidates for multiple functionalization, which has led to their expanding importance in biology and medicine. Recent advances have bolstered hopes that many of the planned fullerene uses may soon be implemented in a variety of fields, including the information technology (IT), diagnostics, pharmaceutical, environmental, and energy sectors. Now that fullerene and its derivatives may be applied directly to biological targets, they show promise as therapeutic agents. The special chemical and physical features of the fullerene core, such as its photodynamic capabilities, are the primary reason for this interest. Recent advances in fullerene derivatives are discussed in the context of their many chemical, physical, and biological functions. In addition to describing fullerenes, this research also delves into their therapeutic applications.**

**Keywords: Structure, Physical, Therapeutic, Chemical, Property, Biological.**

## I.INTRODUCTION

Molecular fullerene is made up of single and double-bonded carbon atoms, making it an allotrope of carbon. As a consequence, many atoms are enclosed in a cage-like structure (a mesh of fused rings) that may be either fully or partly closed. In this configuration, the fullerene molecule may take on a wide variety of forms and sizes, including a hollow spherical shape, an ellipsoid, a tube, and many more. Carbon nanotubes are structures made up of carbon molecules aligned in a cylindrical shape.

Since their discovery in 1985, fullerenes have garnered significant interest across many scientific disciplines. The physical, chemical, and biological characteristics of fullerenes have been the subject of much study, with encouraging results. Inferred advantages in terms of size, hydrophobicity, three-dimensionality, and electrical configurations make them a fascinating topic in medicinal chemistry. Because of their unusual carbon cage structure and the vast possibilities for derivatization, they might be used as a medicinal agent. While carbon spheres aren't very soluble in physiological conditions, that hasn't stopped researchers from learning more about their potential biological uses.

The optical, electrochemical, and physical characteristics of the fullerene family, and C60 in particular, have therapeutic applications in a wide range of medical disciplines. Hydrophobic HIV proteases have a cavity that fullerene can fit into, blocking substrates from reaching the enzyme's catalytic site. A powerful antioxidant, it may also be utilised to neutralise free radicals. However, fullerene may generate large amounts of singlet oxygen when exposed to light. Cleaving DNA is possible via this process and the direct transfer of electrons between the excited state of the fullerene and the DNA bases. Fullerenes have also been used in medication and gene delivery systems. Additionally, they are used as MELDI material for the purpose of serum protein profiling and biomarker development (Bakry et al., 2007)

### Structure of Fullerene

Natural fullerenes are often rather symmetrical structures. Their hexagonally ringed sheet structure is quite similar to that of graphite (cage structure). However, the pentagonal or even heptagonal rings present prevent the sheet from flattening out. Their form determines whether they are called buckyballs or buckytubes. Nanotubes are cylinder-shaped fullerenes.

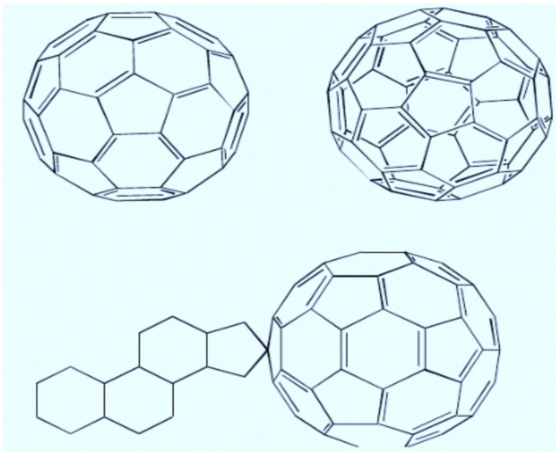

Figure 1: Different Fullerene derivatives

Regardless, the potential number of fullerenes is boundless. Different types of fullerenes exist, including C60, C70, C80, and C90. The amount of carbon atoms in the molecule is a major factor in this. But their primary structure is based on pentagonal and hexagonal rings built according to the guidelines for creating icosahedra.

The arc discharge process is used to synthesise fullerene, and high performance liquid chromatography is used for analysis (HPLC). "At 1000 degrees Celsius, the synthesis process yields C60 and C70, with the concentration rising with increasing pulse time." Organic photovoltaics (OPV), portable electricity, medicine, antioxidants, and biopharmaceuticals are just some of the many potential applications for fullerenes (Jyoti Yadav, 2017).

The scientists have given the newly discovered carbon cluster the name 'Buckminsterfullerene' in honour of architect Richard Buckminster Fuller, whose 1967 dome had the same form as the molecule. In 1996, the three scientists who discovered fullerenes1 shared the Nobel Prize in Chemistry for their groundbreaking discovery due to the widespread interest and excitement the molecule had aroused among researchers. After further investigation, it was discovered that fullerenes occur naturally in interstellar dust and in Earth's geological formations, although at very low concentrations (ppm). Shunga (Russia), Sudbury (Canada), and New Zealand are a few examples.

A fullerene is a huge carbon cage molecule that is the 3-D equivalent of 2-D benzene. Buckminster fullerene (C60) with its spherical arrangement of 60 carbon atoms is the most common kind of fullerene. The truncated icosahedron form of the molecule is reminiscent of a soccer ball, which also has 12 pentagons and 20 hexagons. In accordance with EULER's theorem, which states that a closed structure constructed from pentagons and hexagons must include exactly 12 pentagons, fullerenes have exactly 12 pentagons. Using this criterion, C60, which does not have any adjacent pentagons, is the smallest stable fullerene.

Fullerenes have distinct chemical and physical characteristics due to their three-dimensional structure. In order to modify the characteristics of the novel molecules, chemical functionalization is a simple process.

## II.SIGNIFICANCE OFCHEMICAL PROPERTIES

Fullerenes' carbon atoms are extremely pyramidalized and reactive because of their spherical form. Orbital rehybridization of the sp2 orbitals to sporbitals with a p-character gain causes the conjugated carbon atoms to depart from planarity. Six electrons are sufficient for reversible reduction of C60 and C70 fullerenes. The occurrence of triply degenerate lowest empty molecular orbitals at relatively low energy levels is responsible for this strong electron affinity (LUMOs). Here are a few of fullerene's rudimentary chemical characteristics: -

- Fullerenes are stable, but not totally unreactive.
- In chemical reactions, fullerene can act as an electrophile.
- It acts as an electron-accepting group and is characterized as an oxidizing agent.
- Fullerenes when doped or crystallized with alkali or alkaline earth metals it showcases superconductivity properties.
- Fullerene is ferromagnetic.
- Some fullerenes are inherently chiral.
- It is soluble in organic solvents such as toluene, chlorobenzene, and 1,2,3-trichloropropane.

Fullerenes have a chemical reactivity that is analogous to an electron deficient olefin, leading to the formation of cycloaddition reaction products through addition at a 6,6-ring junction. It has been observed that rearrangements after the first kinetic addition to a 6,6 bond may lead to additions at the 5,6 ring junction.

The allotropes of carbon known as fullerenes have been proposed as a new class of molecules. In contrast to diamond and graphite, this material consists of a hollow carbon cage. C60 spheroidal cage constructions originated from the concept of geodesic domes, which were developed by famous architect Buckminster Fuller. The biological uses of fullerenes are promising, notwithstanding their poor solubility in physiological conditions. C60 and related fullerene compounds have medicinal uses because to their optical, electrochemical, and physical characteristics. Because fullerenes may enter the hydrophobic cavity of HIV proteases, they have the potential to block substrates from reaching the enzyme's catalytic active site. Because of its antioxidant and radical-scavenging properties, it is a useful tool in preventing cell damage. Light exposure also causes significant quantum yields of singlet oxygen formation, which, in combination with direct electron transfer between the excited states of fullerenes and DNA bases, ultimately leads to DNA cleavage. Aside from its usage as a structural component, fullerenes are also a vital part of the gene and medication delivery systems. Fullerenes are intriguing chemicals, and their low toxicity is enough to pique the curiosity of scientists (Gokhale, Madhura & Somani, Rakesh, 2015).

It was thought that fullerenes were inert at first, but it was later discovered that their special cage structure and solubility in organic solvents made them vulnerable to functionalization by addition and redox processes. Buckminster fullerene [C60] and its endohedral and exohedral variants have carved out a special place for themselves among carbon nanomaterials in the fields of medicine, electronics, energy, and water treatment/ conservation (Nimibofa et al., 2018).

## III.PHYSICAL PROPERTIES OF FULLERENES

When exposed to pressures of over 3000 atmospheres, fullerenes may recover their former shape. When compressed to 75% of its original size, a single C60 molecule has an effective bulk modulus of 668 GPa, according to theoretical calculations. Due to this quality, fullerenes are more durable than steel and diamond (160 GPa and 442 GPa, respectively). At normal temperature, fullerenes are the only allotrope of carbon that is soluble in various popular solvents. C60 solutions have been reported to exhibit significant indices of refraction, a dielectric constant of about 4, huge molecular volumes, and a Hildebrand solubility parameter equivalent to 10 cal1/2 cm3/2.

Physical Properties of Fullerene

- Its behaviour and structure depend on the temperature. As the temperature is increased fullerene gets converted into the C70.
- Fullerene structure can change under different pressures.
- Fullerene has an ionization enthalpy of 7.61 electron volts.
- Its electron affinity is 2.6 to 2.8 electrons volts.

Yadav, Bal & Kumar, Ritesh. (2008) fullerene structure, characteristics, and potential uses are discussed. In addition to graphite and diamond, fullerenes are another allotropic carbon substance. In 1985, Harold. W. Kroto, Robert F. Curl, and Richard E. "Smalley made the discovery of these. Having 20 hexagonal rings and 12 pentagonal rings, fullerenes are closed cage structures with icosahedral symmetry." Each carbon atom is sp 2 hybridised and bonded to three others. The 6:6 ring bonds, which may be thought of as 'double bonds,' are shorter than the 6:5 bonds in the C 60 molecule. C-60 is not 'superaromatic' since it has poor electron delocalization because of its tendency to avoid double bonds in the pentagonal rings. Because of this, C 60 quickly interacts with electron-rich species, much like electron-deficient alkenes. The stability of the molecule may be attributed to the geodesic and electronic bonding components in the structure. Organic photovoltaics (OPV) may make use of fullerenes, which are potent antioxidants that react quickly and efficiently with free radicals that cause cell damage and death. Catalysts, purifying water, protecting against biohazards, mobile electricity, automobiles, and medicine are just a few of the many more applications for C 60.

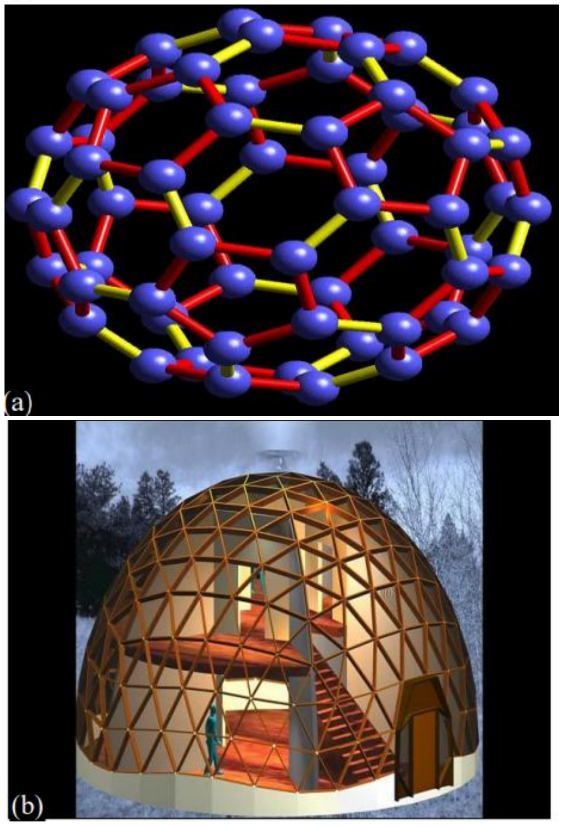


Figure2: (a) A Buckminsterfullerene, (b) A Geodesic Dome.

Macovez, Roberto. (2018) reviews the background information and basic features of binary fullerene cocrystals with a specific emphasis on solvates and salts of Buckminsterfullerene (C60) and hydrates of hydrophilic C60 derivatives. Lattice structure, the existence of orientational disorder and/or rotational dynamics (of both fullerenes and cocrystallizing moieties), thermodynamic parameters such as decomposition enthalpies, and charge transport properties are all investigated. In these binary solid-state systems, the degree of intermolecular interactions may be deduced from both thermodynamic parameters and molecular orientational disorder. Functionalized C60 solid phases and pure fullerite are also compared. Experiments on binary fullerene cocrystals have yielded a number of interesting results, such as the observation of proton conduction in hydrate solids of hydrophilic fullerene derivatives and the production of super-hard carbon materials by applying high pressures to solvated fullerene crystals, both of which are indicative of the presence of molecular rotations.

## IV.THE BIOLOGICAL MECHANISMS DRIVING TOXICITY Of FULLERENE

Numerous researchers have shown that fullerenes may cause toxicity by triggering an inflammatory response and oxidative stress. As a result, it may be feasible to draw generalisations about the processes responsible for fullerene toxicity. So, we'll talk about the mechanisms behind fullerene's toxicity. Further, we will discuss how cellular absorption of fullerenes may increase both clearance and toxicity. Fullerenes' potential genotoxicity and reproductive toxicity will also be discussed.

Many attempts have been made to apply C 60 and its derivatives since since fullerenes were first produced in 1990. In reality, fullerene has several useful biological qualities, such as the ability to suppress HIV-P, cleave DNA with light, protect neurons from damage, prevent apoptosis, and so on. These compounds show promise as novel pharmacophores for structure-activity relationship research in medicinal chemistry, but their poor solubility in biological fluids prevents them from being widely used. Recent efforts to improve the water solubility of C 60 by functionalization have been summarised by Da Ros et al., (2001), as have exploratory research on biological targets. In specifically, DNA photocleavage, antimicrobial activity, and HIV-P inhibition are covered.

There has been a lot of interest in fullerenes across scientific disciplines since since their experimental discovery in 1985. Studies of fullerenes' chemical, physical, and biological characteristics have shown encouraging findings. Fullerenes have the potential to be used as a medicinal agent due to their distinctive carbon cage structure and extensive room for derivatization. So, in this work, Thakral, Seema, and Mehta, R. examine the many ways in which fullerenes might be used in medicine (2006). Fullerenes have several potential medical applications, some of which include as diagnostic agents, free radical scavengers, antimicrobials, and even proteases that can break down HIV.

Since fulleres are a special kind of carbon allotrope, scientists have spent a lot of time learning about their unusual features and considering how they may be used in many fields of technology and medicine. The work by Parambath et al. (2011) highlights several example research connected to such a focus, such as the use of fullerenes for drug-like capabilities and for their improvement in the formulation of known medications, as drug development and formulation have been a key focus in the latter. Possible medicinal uses of fullerenes, such as their use as powerful agents in photodynamic treatment and magnetic imaging, are being considered.

### Fullerene-Mediated Inflammatory Responses

Inflammation has been shown to be induced by a wide range of NPs, leading many to assume that it is a typical reaction after exposure. Since fullerenes are classified as NPs, we must take into account their ability to promote inflammation. In vitro studies have shown that fullerenes may increase the production of proinflammatory mediators including IL-8 and tumour necrosis factor (TNF), suggesting that the inflammatory response may play a significant role in fullerene toxicity. However, in vivo inflammatory-mediated responses are poorly understood and should be the focus of future research.

Studies have shown that fullerene derivatives may be able to inhibit inflammatory reactions. Fulleropyrrolidine-xanthine molecules based on C60 were synthesised by Huang et al. (2008) and then disseminated in cell culture media with 1% dimethyl sulfoxide [DMSO]. The xanthine linkage was thought to be able to dampen inflammatory responses while the fullerene part would operate as a free radical scavenger. J774 macrophage-like cells were treated with the fullerene before being exposed to lipopolysaccharide (LPS), and the fullerene effectively blocked the synthesis of nitric oxide and tumour necrosis factor alpha (TNF) that LPS normally triggers. These results point to the potential for using fullerene derivatives as anti-

inflammatory drugs. The theory needs to be explored further, but additional research is needed.
Treatment with fullerene was tested for its effect on tumour necrosis factor alpha (TNF)-mediated cell death by Harhaji et al. (2008). The mouse L929 fibroblast cell line was shown to be cytotoxic to both THF-prepared C60/C70 and polyhydroxylated fullerene preparations (up to 250 g/ml for 24 hours, distributed in serum-containing cell culture media). Furthermore, a synergistic interaction between C60/C70 and TNF was detected, with the combination therapy being more harmful than the individual treatments. "However, it was shown that functionalized fullerenes gained a protective action when treated with tumour necrosis factor alpha (TNF), suggesting that co-treatment of TNF and polyhydroxylated fullerene might mitigate TNF's harmful impact." Further evidence supporting this discovery was that exposure to C60/C70 boosted TNF-mediated ROS generation and mitochondrial depolarization, whereas polyhydroxylated fullerenes reduced both. It was hypothesised that fullerenes' ability to influence TNF-mediated toxicity was determined by their ability to modulate TNF-mediated ROS generation. It was hypothesised that TNF exposure would increase ROS generation and the cytotoxic response, but that polyhydroxylated preparations would have the opposite effect, acting as a cytoprotectant by blocking TNF's cytotoxicity. It is consequently impossible to generalise about fullerene behaviour and forecast its behaviour, as the research demonstrated by highlighting the fact that two fullerene preparations might behave extremely differently. It's worth noting, however, that THF was used in the C60/C70 sample preparation, which may account for some of the sample's increased toxicity.

It is often believed that NPs cause inflammation, and scant evidence supports this belief; this is especially true for fullerenes. In contrast, fullerenes' anti-inflammatory function has been studied since it may be used in therapeutic therapies. The results show that the inflammatory potential of fullerenes may be affected by factors such as fullerene concentration, fullerene derivative (which, on occasion, was purposely adjusted to incorporate an anti-inflammatory feature), and experimental methodology.

Fullerene-Mediated Oxidative Responses

Scientists have been looking at whether or not fullerenes have the same pro-oxidant potential as NPs because of their propensity to increase ROS production inside cells, hence stimulating the development of oxidative stress.
NanoC60 (0.24-0.24 ppb, or 0.00024-2.4 lg/ml) produced in THF and subsequently distributed in serum-containing cell culture medium was shown to be cytotoxic to many cell lines through increased reactive oxygen species (ROS) generation, lipid peroxidation, and membrane damage by Sayes et al., 2005. (dermal fibroblasts, hepatocytes, and astrocytes). Lactate dehydrogenase (LDH) release and increased permeability of fullerene-exposed cells to dextran are both indicative of compromised cell membrane integrity. The fact that fullerene-mediated cytotoxicity could be suppressed by administering the antioxidant ascorbic acid provided more evidence that reactive oxygen species were involved. The described results are frequently incongruous and imply that fullerenes may generate pro-oxidant effects under certain circumstances, but not under others; this is likely to be determined by the fullerene in question, the cell type being researched, and the experimental apparatus.

Antioxidant Properties of Fullerenes

Some fullerene derivatives have been called ‘radical sponges’ because to the emphasis placed on studying C60's potential free radical-scavenging ability (Xiao et al., 2006). This is motivated by the realisation that there is potential to use fullerene administration to shield against radical-mediated damage caused by toxicant exposure or a variety of disease conditions.
The free radical-scavenging activity of C60 is thought to be the driving force behind the protective effect found by Gharbi et al. (2005), who injected C60 (0.5-2 g/kg) into the ip veins of rats to prevent carbon tetrafluoride-mediated liver injury. It was also hypothesised that C60's antioxidant capability is proportional to its degree of dispersion. Antioxidant behaviour of fullerenes is enhanced inside water-soluble forms, as the authors hypothesised, since aggregates of C60 will not display antioxidant capabilities owing to the lack of availability of the unsaturated bonds inherent within the molecule's structure.
Several fullerene derivatives were tested for their free radical-scavenging activity and, by extension, their cytoprotective effects in a separate research by

Yin et al. (2009). (dispersed in serum containing cell culture medium).

## V.APPLICATIONS OF FULLERENEIN DIFFERENT AREAS

The unique physical and chemical properties of fullerenes has led many researchers to explore the application of this molecule and it's functionalized derivatives in various areas such as medicine, photovoltaics, gas adsorption/storage, pharmaceuticals just to mention a few.

Medical Application

Size, Hydrophobicity, electronic configuration and three - dimension ability is some of the most alluring characteristic of fullerene which has brought them to the front burner of medical chemistry. In spite of obvious solubility challenges their exceptional carbon cage structure and vast scope for functionalization make fullerenes standout as potential therapeutic agents (Iwamoto & Yamakoshi, 2006).

Antioxidant/Biophamaleuticals

Fullerenes react readily with free radicals because of the presence of large amounts of conjugated double bonds and low lying Lowest Unoccupied Molecular Orbitals (LUMO), it has been reported that about 34 methyl radicals have been added onto a single C60 molecules as such it is considered the world's most efficient radical Scavenger (Gharbi, Pressac, & Hadchouel, 2005).

Antibacterial/Antimicrobial Activity

Antibacterial properties of hydrophilic fullerene derivatives such fullerols and amino fullerene have piqued interest in their potential use in water purification systems (Kang, Mauter, & Elimelech, 2009). Multiple hydroxyl groups, carboxyl groups, and glycolic oxide groups attached to C60 have been demonstrated to initiate photodynamic cycotoxicitly against pathogenic microbes, including multi-antibiotic-resistant bacteria, according to published reports (Thota et al., 2012). C60's propensity to create reactive oxygen species (ROS) such as singlet oxygen and superoxide through photosensitization when interacting with organic solvents is largely responsible for its biocidal effect (Das et al., 2017).

Antiviral Activity

Antiviral potentials exhibited by fullerene derivatives have been linked to their matchless molecular cage structure and antioxidant property. An investigation revealed that fullerene derivatives could restrain and form a complex with HIV protease (Barras, Khanal, & Boukheroub, 2015). Reports have also shown that, fulleropyrolidines bearing two amino groups were active against HIV - I and HIV – 2.

Diagnostics

An endofullerene is created when a metal ion is placed into a fullerene cage, and this endohedral metallofullerene cage has the potential to behave as an isolation chamber that keeps reactive atoms from the biological environment (Dorn & Fatourus, 2010). Gadolinium encapsulated endohedral metallofullerenes (EMFs) are a promising new use for EMFs; they have been called 'top prospects' for next-generation MRI contrast agents (Toth, 2012). Biodistribution studies have also shown that metallofullerols are concentrated in microphages, suggesting that these compounds are specifically targeted to microphage-rich tissues and have the potential to be highly useful chemotherapic agents in the treatment of bone cancer and leukaemia (Azzam & Domb, 2004).

Drug Delivery

Fullerenes have the potential to be used as drug carriers for cellular delivery due to their high biocompatibility, selectivity in targeting, and ability to release pharmaceuticals at a predetermined rate. Attaching hydrophilic species to fullerenes makes them water soluble, making them ideal for medication and gene cellular delivery (Foley et al., 2002). Because functionalized fullerenes may pass through cell membranes and attach to mitochondria, their drug delivery can be controlled to be gradual, allowing for optimum therapeutic effect. DNA-functionalized fullerenes have been shown to be much more successful than lipid-based vectors currently on the market (Bottary, Swanzes, Trukhina, & Torres, 2011).

## VI.USE OF FULLERENE AS THERAPEUTIC AGENTS

There have been several efforts to investigate novel delivery methods with the introduction of new medications. To make up for the shortcomings of standard practise, targeted delivery systems are a sought-after intervention. "Many different nanoparticles have been suggested and researched in an effort to make this concept a reality." To effectively transport therapeutic chemicals, these nanoparticles will need to interact favourably with biological surroundings and traverse cell membranes. The fullerenes were one of the first classes of carbon-based nanoparticles used in targeted delivery. Because of their unusual structure and desirable features, fullerenes may interact with cells and their surrounding environments. This brief article focuses on recently produced fullerene derivatives and their potential as cutting-edge delivery methods for pharmacological uses (Kazemzadeh, Houman & Mozafari, Masoud, 2019).

Therapeutic effects of pure C60 fullerene aqueous colloid solution (C60FAS) on the function of the rat soleus muscle after ischemic injury were discussed by Nozdrenko et al. (2017). These effects were found to vary with the stage of the general pathogenesis of the muscular system and the method of administration C60FAS in vivo. Correction of speed macroparameters of contraction for ischemic muscle injury was shown to be best with intravenous infusion of C60FAS. When C60FAS is injected intramuscularly, it has a strikingly restorative effect on muscles engaged in activities where maximal force responses or sustained contractions contribute to increased muscle exhaustion. C60FAS has promise as a therapeutic agent for the prevention and repair of ischemic-damaged skeletal muscle function, as shown by an analysis of the content concentration of creatine phosphokinase and lactate dehydrogenase enzymes in the blood of experimental animals.

According to a study by Fernandes et al., (2022), cancer is the leading cause of death worldwide. The non-specific targeting of currently available treatments means that they come with serious adverse effects. As a result, the healthcare system need an alternative that is very effective but has few adverse effects, and which can also be targeted to a particular area of the body and repeated reliably. As a result of fullerenes, this is now a realistic goal. The physicochemical and photosensitizer characteristics of fullerenes are unparalleled. This article focuses on the use of C60 fullerenes in cancer therapy and examines their creation, functionalization, mechanism, characteristics, and potential applications. The paper also covers the circumstances, toxicity profile, and future prospects that affect fullerene activity.

## VII.CONCLUSION

While fullerenes were formerly thought to be inert compounds, their distinctive cage structure and solubility in organic solvents have shown that they are really rather amenable to exodehedral and endohedral functionalization. Adducts formed by addition processes are called exohedral, whereas those formed via redox reactions, such as polymer films, are called endohedral. The key to unlocking the vast potential of this third allotrope of carbon is a firm grasp of the rules guiding the functionalization of the most prevalent fullerene (C60). Functionalized fullerenes have potential in methane storage, catalysis, and environmental studies, however this area needs further attention.

Its action in several sectors may be attributed to both the hydrophobic spheroid and the radical sponge property of fullerene. "There is a unique redox chemistry associated with fullerenes, which allows them to be reduced by up to six electrons in a reversible manner." Together with the minimal toxicity shown in fullerenes so far, these facts are enough to motivate chemists and biologists to pool their resources and rigorously explore the biological aspects of these interesting molecules. Anticancer medication delivery systems using photodynamic therapy, HIV treatments, and cosmetics to slow down human skin ageing are just some of the many possible commercial uses that have resulted from the recent surge in global research and development efforts. In the future, industry will benefit from the fullerene field's discoveries. The high cost of manufacturing fullerenes has historically been the primary restraint on the fullerene market's expansion. This newfound affordability will enable a wide variety of previously unimaginable uses. In addition, several marketed fullerene uses may be found in industry.

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