C60 Fullerene

Fullerene-C60 is a non-toxic antioxidant 100–1000 times more active than vitamin E. Although C60 itself is not at all water soluble, many highly water soluble fullerene derivatives have now been prepared.

Related terms:
Carbon Atom, Titanium Dioxide, Graphene, Fullerene, Graphite, Heterocyclic Compound, Molecule, Compound Isomer

Learn more about C60 Fullerene

Safety issues relating to nanomaterials for construction applications

M Spitzmiller, ... R Damoiseaux, in Nanotechnology in Eco-Efficient Construction, 2013

C60 fullerenes and their derivatives

C60 fullerenes may be respired during the preparation process, causing lung inflammation (Park et al., 2010). In addition to their use as raw nanomaterials, these fullerenes are often suspended as water-stable aggregates. The resulting fullerene solution has been shown to have broad antimicrobial potential (Lyon et al., 2005, 2006). While there have been hypotheses that this cytotoxicity is mediated by oxidative stress from ROS, recently it has been shown that direct cell membrane oxidation from C60 contact is likely responsible (Lyon and Alvarez, 2007; Lyon et al., 2008). In eukaryotes, this oxidative stress is also responsible for cell death, leading to lipid peroxidation (Oberdörster, 2004; Sayes et al., 2005). Derivatives of C60 fullerenes, such as fullerol and carboxyfullerene, can cause cytotoxicity by physical membrane damage (Tsao et al., 2002) as well as by oxidative routes (Faruk and Matuana, 2008).
1.5.1 Fullerene

Fullerene $C_{60}$ (buckyballs or buckminsterfullerene) is a nanostructured allotrope of carbon (Fig. 1.11) that has been of significant interest to various fields of science and engineering. Fullerene and its derivatives have enormous potential in materials science owing to their unique physical and chemical properties. Although fullerene was discovered in 1985 by Kroto et al., its preparation process is still not yet fully understood. There are several theories for the formation of fullerene derivatives, such as fullerenes $C_{60}$ and $C_{70}$; laser evaporation of graphite was used by Kroto and colleagues. They were discovered $C_n$ clusters ($n \geq 20$) of which the most usual were found to be $C_{60}$. In 1985, the Nobel Prize in Chemistry was awarded to Kroto Curl and Smalley for their discovery of fullerenes [46]. Thereafter, other desired fullerenes, such as $C_{76}$, $C_{80}$, $C_{240}$, etc., were synthesized from large numbers of carbon atoms. Since their discovery nearly three decades ago, an enormous number of research articles have considered the nanoheterostructures of fullerenes. Several efficient and less costly methods for producing fullerene nanoheterostructures have been developed [47, 48]. $C_{60}$ and its derivatives have tremendous potential in materials science due to their unique physicochemical properties [49]. Lately, $C_{60}$-based nanostructures, including nanotubes, nanorods, and nanosheets have attracted unique attention in the fields of nanoscience and nanotechnology [50]. The appearance and use of low-cost fullerenes represents the way forward for further studies and practical applications.
Fig. 1.11. Nanoallotropes of carbon.

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**An Introduction to Green Nanotechnology**

Mahmoud Nasrollahzadeh, ... Monireh Atarod, in *Interface Science and Technology*, 2019

2.3.1.1 Fullerenes
 Fullerene (C\textsubscript{60}) is a carbon-based molecule that is spherical in morphology and made up of carbon atoms held together via sp\textsuperscript{2} hybridization. Generally, the other fullerences (0D), such as C\textsubscript{76}, C\textsubscript{80}, C\textsubscript{240}, etc, are synthesized from larger numbers of carbon atoms. Fullerenes are comprised of between 28 and 1500 carbon atoms that form spherical structures. Single-layer fullerenes have diameters up to 8.2 nm while multilayer fullerenes have diameters of between 4 and 36 nm. Over the past few years, solar cells have attracted much attention due to their important role in the production of energy. Nowadays, fullerene derivative [6,6]-phenyl-C\textsubscript{61}-butyric acid methyl ester (PC\textsubscript{61}BM), plays the role of an electron transport layer for high-efficiency p-i-n planar heterojunction perovskite solar cells. Recently, Xie et al. used a solution of pristine fullerenes (C\textsubscript{60} and C\textsubscript{70}) as electron transport layers. They proposed replacing the PC\textsubscript{61}BM in perovskite solar cells. Fig. 2.1 (left) provides SEM images of a CH\textsubscript{3}NH\textsubscript{3}PbI\textsubscript{3} film on FTO/PEDOT:PSS substrate. Large grain sizes and pinhole-free CH\textsubscript{3}NH\textsubscript{3}PbI\textsubscript{3} films are depicted in Fig. 2.1 (left). CH\textsubscript{3}NH\textsubscript{3}PbI\textsubscript{3} layer spin-coating with an optimized thickness of ~ 50 nm is responsible for the difference ratios of C\textsubscript{60} and C\textsubscript{70} as ETLs. Finally, they thermally evaporated an Ag electrode. As shown in the cross-sectional SEM image in Fig. 2.1 (right), the thicknesses of the perovskite layer, the pristine fullerene layer, and the Ag electrode was about 270, 50, and 100 nm, respectively [11].
In 2016, Porfyrakis et al. reported the synthesis of a series of fullerenes and carbon nanotubes and investigated the effect of the addition of copper nitrate. Copper nitrate acts as a doping agent during arc-discharge vaporization of Gd-doped and Nd-doped rods. Gd-1X has a low number of nanofibers, with diameters of 100 nm, embedded in a carbon matrix [12]. Based on a TEM image of a GdCu-1A sample, multiwalled nanotubes (MWNTs) were embedded in an amorphous carbon matrix.
In addition, the average outer diameter of the MWNTs inorganic nanoparticles was about 20 nm. Dark particles were clearly present in the carbon matrix and were most probably gadolinium carbides [12]. Endohedral metallofullerenes, due to their functional properties and potential applications, attracted significant interest in the field of nanomaterials science. For example, Nakayama et al. investigated the thermal stability and electron energy of Sc$_3$N@C$_{80}$ fullerenes, inserted inside carbon nanotubes (CNTs). Fig. 2.2A shows a TEM image of Sc$_3$N@C$_{80}$ fullerenes encapsulated in single-walled nanotubes (SWNTs). The TEM image shows many amorphous carbons and fullerenes, on the walls of carbon peapods, as impurities. In addition, clearly almost all SWNTs were filled by fullerenes. Chemical treatments or annealing at high temperatures are suitable techniques for removing such impurities. Fig. 2.2B shows clean carbon peapods. TEM images confirmed the cleaning process removes the majority of amorphous carbon and fullerenes from the walls of CNTs [13].
Fig. 2.2. (A) TEM image of $\text{Sc}_3\text{N}@\text{C}_{80}$ fullerenes encapsulated in SWNTs by thermal heating at 650°C for 5 h. (B) TEM image of clean carbon peapods.

(Reproduced with permission from Fallah A, Yonetani Y, Senga R, Hirahara K, Kitaura R, Shinohara H, Nakayama Y. Thermal/electron irradiation assisted coalescence of
Applications of Ball Milling in Supramolecular Chemistry


8.2 Complexation of Fullerenes

Complexation of fullerene C₆₀ with β-cyclodextrin was attained by employment of high-speed vibrational milling (HSVM) by Komatsu et al. (Scheme 8.6) [14]. Fullerene C₆₀ was complexed within 10 min milling with fourfold excess of cyclodextrin, forming a 1:2 complex 25 with a bicapped structure. The solid-state mechanochemical technique was found to be more effective for complexation in contrast to conventional solution phase (reflux, 24 h). Complex 25 exhibits the highest solubility in water than the complex prepared by other methods. It was found that shorter (5 min) or longer (20 min) milling afford complex which is soluble in water to lesser extent. This high-energy milling was more effective than complexation by classical ball milling which was carried out for about 20 h (Fritsch Pulverisette 701, agate vial 50 mL, ball 15 mm) [15].

Scheme 8.6. Fullerene complexation with cyclodextrin.

Equally effective was the complexation of C₇₀ by HSVM (10 min, C₇₀:β-cyclodextrin 1:8), while the other functionalized C₆₀ derivatives afforded water-soluble 1:1 complexes, since functional groups prevent the formation of the bicapped 1:2 complexes. By mechanochemical treatment, fullerene C₆₀ also complexes with sulfocalix[8]arene (10 min, equimolar amounts), and the obvious advantage of the solid-state complexation is illustrated by the complexation of sulfocalix[8]arene with fullerene dimer (also prepared by mechanosynthesis, see chapter: Applications of Ball Milling in...
Nanocarbon Material Synthesis. Dimer is hardly soluble in most common **organic solvents**, but the mechanochemical treatment of an equimolar mixture of sulfocalix[8]arene and fullerene dimer for 10 min afforded bicapped complex, which is about twice more soluble in water than in commonly used ODCB.

Besides ß-cyclodextrin and sulfocalix[8]arene, Geckeler has found that C₆₀ forms a complex with cucurbit[7]uril in mechanochemical conditions (Scheme 8.7) [16]. Retsch MM200 mill was employed, in stainless steel capsule (inner diameter 18 mm) and ball (12 mm) at 20 Hz. Irrespective of the molarity of two components, a supramolecular 1:1 complex 27 was formed through noncovalent binding after 4 h in 77% yield, which was more effective than solution preparation (96 h, 55%).

![Scheme 8.7. Fullerene complexation with cucurbit[7]uril.](image)

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**Superlubricity of Molybdenum Disulfide**

Jean-Michel Martin, in *Superlubricity*, 2007

### 13.8 ULTRALOW FRICTION BY MoS₂ NANOPARTICLES

Following carbon **fullerenes** (C₆₀) and **carbon nanotubes**, hollow nested (or onion-like) **nanoparticles** made of **metal dichalcogenides** have been synthesized as a response of the size-decrease need and replacement of organic compounds, generally environment-sensitive. Basically, a metal-doped powder in nanometer-size is converted into an inorganic fullerene-like (IF) structure by reacting it with H₂S at high temperature and turbulent **flow regime** in a reactor. Tenne et al. [31] have successfully synthesized IF-MoS₂, IF-WS₂ and more recently IF-NbS₂. It was shown that IF-MoS₂ and IF-WS₂ demonstrate excellent tribological properties as **solid lubricants** and **additives** in oil and **greases** and also various coatings [32]. A high resolution TEM picture of IF-MoS₂ nanoparticles shows that the distance between two consecutive sheets (c/2 = 0.63 nm) is in good agreement with the 2H–MoS₂ **crystal** structure. The low quantity of oxygen content of IF-MoS₂ was evidenced by XPS and EELS in the TEM. This can be well explained by the absence of crystal edges.
in the onion-like structure of the nanoparticles. IF-MoS$_2$ can provide ultralow friction when used as an additive to a synthetic base oil in boundary lubrication conditions [33]. The explanation of low friction of onion-like structure has first been attributed to a rolling mechanism, like in a nanometer-scale ball bearing. However, it has been shown by TEM that most of nanoparticles entering the contact area are flattened at the exit, suggesting that friction finally occurs between MoS$_2$ nearly flat external planes. In some cases, tearing and unwrapping of fullerene generates some MoS$_2$ singles sheets [34]. These single sheets are known to lubricate in the ultralow regime. What concerns superlubricity of IF-MoS$_2$ is not clear at the moment. We did not observe superlow friction in our conditions, although the purity of the MoS$_2$ material should allow superlubric state to be reached, according to Hirano’s model. However, Chhowalla observed a case of superlow friction with IF-MoS$_2$ coatings [34].

### 13.8.1 Nanotribology on MoS$_2$ Crystals

The question of superlow friction of MoS$_2$ in nanotribology is not yet elucidated. Observation of a superlubric state has already described by Hirano by sliding W(100) against Si(100) in a dedicated UHV/STM [35]. Dienwiebel, in his Ph.D. thesis, evidenced the superlubric state of graphite in UHV in a friction force microscope. What concerns MoS$_2$, Miura [36] studied the friction between two MoS$_2$ flakes. He found that the Amontons–Coulomb law was satisfied and that the friction coefficient between MoS$_2$ surfaces along the [1010] direction of the MoS$_2$ (0001) surface was superlow at 0.003.

> Read full chapter

## Carbon nanostructures

Lei Yang, in Nanotechnology-Enhanced Orthopedic Materials, 2015

### 5.2.4 Orthopedic medical application of fullerenes

The potentials of fullerene (C$_{60}$, not water soluble) and its derivatives (maybe water soluble) for supporting bone cell growth and treating arthritis have been studied. Grausova et al. [80] investigated osteoblast-like MG63 cell adhesion and growth on continuous or micropatterned fullerene films deposited on glass coverslips. Results indicated cell adhesion and proliferation activities on all kinds of fullerene films were similar to those on tissue culture polystyrene (TCPS) dishes, and region-selective cell adhesion and growth were observed on the grooves of the micropatterns. Similar results were reported on binary fullerene/titanium composites (C$_{60}$:Ti = 1:1) [81]. Gonzalez et al. [82] designed
a fullerene-based material, C\(_{60}\)(OH)\(_{16}\)AMBP (4,4-bisphosphono-2-(polyhydroxyl-1,2-dihydro-1,2-methanofullerene(60)-61-carboxamido)butyric acid), to specifically target HA in bone tissues, showing the promise of fullerene derivatives for treating bone-related diseases. Fullerene functionalized with diphosphonate groups were expected to possess the same ability to selectively target bone tissues [83]. Yudoh et al. conducted a series of studies on using water-soluble fullerene to treat arthritis [84–86]. Their studies used water-soluble fullerene as an oxygen free radical scavenger to reduce articular cartilage degeneration and inhibit osteoclast differentiation and bone destruction. However, although fullerene has exhibited the strong potentials in orthopedic medical field, it is important to be aware of its possible toxicity problems. There are many studies conducted to reveal the possible health risks of fullerene [87–89], which will be covered in Chapter 9.

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Growth and characterisation of fullerene/GaAs interfaces and C\(_{60}\)-doped GaAs and AlGaAs layers

Jiro Nishinaga, in Molecular Beam Epitaxy, 2013

24.1.1 Introduction

The discovery of fullerene C\(_{60}\) [1] and its synthesis on a microscopic scale [2] have stimulated research efforts, and extensive investigations of its physical and chemical properties have opened a device application field such as thin film transistors and solar cells. C\(_{60}\) molecules are highly symmetric as shown in Figure 24.1 and crystallize into a face-centred cubic structure on crystalline substrates such as Si and GaAs, despite the large lattice mismatch between C\(_{60}\) and the substrates [3–10]. Reflection high-energy electron diffraction (RHEED) is used to observe the growth and surface conditions of semiconductor films, and RHEED intensity oscillation enables dynamic effects to be investigated [11]. Organic materials tend to be decomposed by electron beam irradiations [12]. But C\(_{60}\) molecules have a stable structure, and the C\(_{60}\) crystal growth may not be influenced by RHEED measurements. In this work, to investigate the growth mechanism of C\(_{60}\) layers, we observe RHEED intensity oscillations during C\(_{60}\) epitaxial growth on GaAs substrates by MBE, and clear RHEED intensity oscillations have been successfully observed [13,14]. The frequencies of the oscillations increase proportionally with the C\(_{60}\) flux and coincide well with the growth rates of C\(_{60}\) layers obtained from the film thickness. This suggests that C\(_{60}\)
layers grow by layer-by-layer mode, as has been observed with growth of GaAs and other semiconductor materials.

FIGURE 24.1. Structure model of a C\textsubscript{60} molecule.

Next, we discuss the fabrication of nanoscale structures such as quantum wires and dots using C\textsubscript{60} crystals. Since C\textsubscript{60} films are very fragile and chemically unstable due to weak binding energies, conventional techniques such as etching and ion milling are not acceptable for nanoscale fabrication processes. Area-selective epitaxy makes it possible to achieve damage-free fabrication. Therefore, we have carried out area-selective epitaxial growth of C\textsubscript{60} crystals on GaAs (111)A, (111)B and (001) substrates with nanoscale open areas by using SiO\textsubscript{2} mask. These structures are formed by electron beam (EB) lithography. The grown structures of C\textsubscript{60} crystals and the surface morphology are investigated by scanning electron microscopy (SEM) and atomic force microscopy (AFM) [9].

> Read full chapter

**Analysis and Risk of Nanomaterials in Environmental and Food Samples**

Troy Benn, ... Paul Westerhoff, in *Comprehensive Analytical Chemistry*, 2012

Abstract
Combustion processes can form fullerenes ($C_{60}$). Therefore we investigate the occurrence of $C_{60}$ in various atmospheric environments. The detection and quantification is achieved with the highly specific and sensitive method of liquid chromatography coupled to mass spectrometry following solvent extraction of the samples. $C_{60}$ was detected in the air particulates of a parking garage and the exhaust soot of a diesel truck. These results would indicate that fullerenes are incidentally produced from combustion processes and become associated with atmospheric particulate matter. However $C_{60}$ is susceptible to atmospheric oxidation processes. In particular ozonation tests on solid $C_{60}$ confirm the production of fullerene-based compounds such as $C_{60}O$. Such oxidation and alteration of the molecular structure of the fullerenes would explain the low ambient concentrations observed respectively the inability to detect $C_{60}$ in ambient air in many locations, further away from potential emission sources. These results have significant policy implications including considering incidental sources of $C_{60}$ in addition to engineered $C_{60}$ added to commercial products, and understanding environmental oxidation processes for $C_{60}$ in conjunction with quantifying transformation products.

> Read full chapter

**Biological activity of pristine fullerene C60**

L.B. Piotrovsky, in *Carbon Nanotechnology*, 2006

**4.2. Water-soluble complexes with polymers (or inclusion complexes)**

Various methods for dissolving fullerene $C_{60}$ in water using various hydrophilic organic compounds were developed in order to overcome its insolubility in this media (for reviews see [8,9,13]). Among them it is necessary to mention the inclusion complex $C_{60}$/β-CD (β-cyclodextrin) $C_{60}$ [58], inclusion of fullerene $C_{60}$ into liposomes [59] and the complex with polyvinylpyrrolidone ($C_{60}$/PVP complex) [60].

The inclusion complex $C_{60}$/β-CD (1:2) was prepared by boiling water solution of β-CD with fullerene $C_{60}$ [58]. As we know, this inclusion complex is a rare example when it was undoubtedly shown that a fullerene molecule is in isolated nonaggregated state but practically nothing is known about the biological properties of this complex. At such shielding of fullerene core as in this complex, the main input in the biological activity is defined by the host molecules. However, it was shown both in physical and biological experiments [28,61] that in this complex in particular fullerene possesses photodynamic properties, while free radicals (e.g. $\cdot OH$) react exclusively with the
macromolecular host ⊙-CD [28]. In the case of the transfer of fullerene C₆₀ into the aqueous phase by inclusion into liposomes, it shows antioxidant activity similar or even higher than natural antioxidant vitamin E [59].

The biological properties of C₆₀/PVP complexes with fullerene concentration ~0.8 wt.% (with which it is possible to obtain aqueous solutions with the concentration of C₆₀ up to 4.1 x 10⁻⁵ M) can be studied much better [60]. The preparation of this complex with higher content of fullerene (1.1–2.7 wt.%) was described in [62]. This complex was already examined in several in vitro biological tests [60,63–67]. However, physicochemical properties of this complex are investigated to be much worse. This complex is formed by weak donor-acceptor interactions [68]. The interactions between C₆₀ and polymer vehicle is not very strong, and fullerene can be easily extracted by toluene from aqueous solution. According to the data, ¹³C-NMR in D₂O in the complex significantly changes the electronic state of the carbon atoms C(1) and C(4) of pyrrolidone cycle and C(5) of the monomeric unit of PVP, nearest to the nitrogen atom [69]. C₆₀/PVP complex, as it was shown by static and dynamic light scattering, forms aggregates with high molecular masses in aqueous solutions [70,71].

The degree of aggregation of fullerene molecules in this complex seems to be low, but it was not determined. This property of fullerene C₆₀ can be monitored, for example, by UV–VIS spectrophotometry. In the range of 320–350 nm, the clustering causes the bathochromic shift of the absorption band with the decrease of extinction coefficient [72]. The analyses of several dozens of UV spectra of C₆₀/PVP complexes, which differ in the content of fullerene and the molecular mass of PVP, shows that the use of PVP with low molecular mass leads to a low degree of association of fullerene molecules in the complexes. For samples with low association, the band is at 331–333 nm, whereas for the other ones it is shifted to 340 nm. Antibasis decreases the values of extinction coefficient (from ~1.0x10⁻⁵ to ~0.4x10⁻⁵ M⁻¹ cm⁻¹). Such complexes can be prepared only with a relatively low content of fullerene (about 0.1–0.2 wt.% to PVP mass) and PVP of low molecular mass (10,000 Da). The degree of association of fullerene molecules in such preparations changes in time during storage for about several months. Certainly, it is not good that fullerene concentration in C₆₀/PVP complexes is rather low (usually ~0.5–0.6 wt.%), but let us remind ourselves that the effective antiviral dose of fullerene itself in the complex is also not high. The active quantity of fullerene, calculated neglecting the polymer vehicle, against the influenza virus is about 7 μM [73].

At the beginning of the studies of fullerene action on influenza virus reproduction, it seemed that the mechanism of fullerene action will be similar to that of lipophilic antiviral drug derivatives of such framework compounds as adamantane [74]. Though the inhibitory activity of the complex is comparable to the antiviral activity of such reference as anti-influenza drug such as rimantadine, there are
distinct differences. First of all, C₆₀/PVP complex did not specifically inhibit any stage of the virus replication cycle, including absorption [75]. The complex is active, in contrast to rimantadine, against both types of influenza virus (A and B), as well as other RNA- and DNA-containing viruses (e.g. herpes simplex and human parainfluenza virus) [76]. It was proposed that C₆₀/PVP complex interferes with the late membrane-dependent stages of morphogenesis of enveloped viruses and so it can be classified as membranotropic antiviral compound [77]. C₆₀/PVP complex influences the morphology of influenza virions predominantly in light-independent manner [53]. Some virions in C₆₀/PVP-virion mixture look like the aggregates with polymer complexes (Fig. 4). It is possible to assume that this image corresponds to the moment of the fusion between the complex and the virion. The fraction of such particles was not large (about 1–3%), this can be the evidence of rather quick interaction of the complex with virions [78].

![Figure 4. TEM image of fusion of C₆₀/PVP complex with influenza virion envelope. Scale 100 nm.](image-url)

On the basis of these data it is possible to speculate that fullerene C₆₀ attached to the polymer vehicle by weak donor-acceptor bonds, can easily move from the complex to the lipid bilayer of the envelope of virion. The transition of fullerene molecules into the lipid bilayer was shown directly with the use of erythrosine as a probe, while pyrene as a probe showed that the fluidity of membranes increases [79].

The obtained data proved the conclusion made earlier about the membranotropic mechanism of antiviral action of C₆₀/PVP [77]. From this point of view the most vulnerable stage in the cycle of influenza virus reproduction is budding, because at this stage the fluidity of the lipid bilayer and the ability of viral glycoproteins to form patches with the regular structure are of great importance [80]. So, the penetration of fullerene molecules into the membrane will change its properties, and will disturb the assembly of virions (Fig. 5A). When the fluidity of the cell membrane increases, the processes of the virion assembly proceed wrongly and damage the noninfectious particles formed (Fig. 5B).
It is not surprising that owing to high lipophilicity of fullerene the penetration of its molecules into membrane, their interactions with bilayer components will lead to the damage of the regular structure and to the formation of the pores in the virion envelope. However, it can be possible only in the case of single fullerene molecules or low associated aggregates, which are smaller than the membrane thickness (5 nm). However, the small increase of virucidal effect of C$_{60}$/PVP complex during illumination [78] allows us to suppose that there is also the input of the second, light-dependent mechanism [81].

> Read full chapter

### Magnetic Properties of Novel Carbon Allotropes

A.V. Rode, ... B. Luther-Davies, in *Carbon Based Magnetism*, 2006

#### 2.1 Two-dimensionally Polymerised C$_{60}$ Molecules

The polyhedral molecules of fullerene, C$_{60}$, undergo cross-linking reactions when annealed at pressures of a few GPa and temperatures of 300–1100K to form a variety of crystalline polymers with layered structures. These polymerised fullerenes (poly-C$_{60}$) demonstrate ferromagnetic behaviour only when prepared in a relatively narrow range of synthesis conditions. A pressure-temperature diagram has been produced that shows systematic variation in the non-equilibrium products that can be synthesised by annealing of C$_{60}$ fullerene under different conditions [33]. The synthesis conditions for magnetic poly-C$_{60}$ cross-linked fullerene synthesis field lies
within 100K of the upper temperature limit for the synthesis of this structure [16].
At higher temperature, the polyhedral carbon cages of fullerene break open further
to form “partially graphitised” layer structures. This indicates that the process of
formation of a ferromagnetic phase may be related to the occurrence of the defects
due to cage opening. It is also feasible that the weak bonds between polyhedra are
readily broken, and can act as the spin centres [34].

It has been shown to be possible that the polymerisation of fullerene cages can
take place via a sequence of Stone-Wales transformations – very local concerted
rearrangements of atoms such as the reconnection of two adjacent 6-rings as a
5-ring and 7-ring (Fig. 2). As the polyhedral cages are opened, large rings (e.g.
11-gons) are formed [7, 24]. The zigzag edges of these rings are known to be
associated with magnetism in graphene ribbons. Furthermore, the formation of
adjacent large rings tends to change the local Gaussian curvature of the structure
from positive in the close buckyball polyhedron to negative in the saddle-shaped
regions between cages.

Fig. 2. Simple example of a Stone-Wales rearrangement, converting graphene
6-rings (a) into mixture of 5- and 7-rings (b).

The magnetic ordering in selected metastable isomers of C_{60} with partly opened
cages was recently theoretically investigated using the spin-polarized density-func-
tional formalism [24]. Several carbon nanostructures, which could be described as broken fullerene cages with specified arrangements of under-coordinated carbon atoms, were identified as potential molecular magnets. Calculations showed that a zigzag arrangement of edge atoms in the defective cage stabilised dangling bonds, which in turn led to magnetic instabilities in isolated molecules and even ferromagnetism in the solid made of partially opened C_{60} cages. However, these calculations did not identify what specific defect structure(s) provided the mechanism of long-range magnetic coupling.

The possibility of magnetic centres arising in defective polyhedral cages was examined in a study that modelled poly-C_{60} using a combination of reactive force field molecular dynamics and hybrid-exchange density functional theory [35]. The model was used to generate potential defect structures and characterise their magnetic ground states. A large number of local defect structures were found to result in local moments. One particularly common structure defect type in this study, resulting from anisotropic strain, is reminiscent of a vacancy-adatom pair in that one atom of a C_{60} cage is forced out to become an inter-cage bridge, leaving an 11-ring hole in the cage. A vacancy-adatom pair on graphite had already been shown to be strongly magnetic (0.45 \mu B/adatom) by the calculations of [36]. The defect of [35] resulted in no net magnetization since spins were coupled via equal numbers of competing antiferromagnetic and ferromagnetic pathways. This suggests that ferromagnetism could be obtained if the coupling strengths of these pathways were perturbed, or if a different defect geometry were involved. Hybrid Density Functional Theory calculations showed that it was particularly favourable for hydrogen to bind at one of the three types of spin centre in this particular defect, and that the perturbation introduced by hydrogen quenched the antiferro coupling pathway selectively, leading to ferromagnetism with moment 3\mu B per cage. The experimental part of the study [35] analysed a sample of ferromagnetic poly-Cm for hydrogen content using inelastic neutron scattering. The presence of hydrogen was confirmed (H/C_{60} = 17%), at a level comparable with that predicted for the observed magnetisation for this model (H/C_{60} = 11%, 0.34 \mu B per polyhedral cage). It is possible that structures which allow greater spin delocalisation or a greater degree of inter-polyhedral linkage would show significantly larger inter-cage couplings.

It is clear from [35] that in some samples of poly-C_{60}, at least, ferromagnetism is a consequence of partial hydrogenation of the sample. Caution regarding magnetism in impurity-free poly-C_{60} is also suggested by [ref. 12 in the paper, to be published], which showed that in the periodic model for poly-C_{60} proposed in [37] where a carbon atom is removed from each C_{60} cage, the magnetic moments localized on each cage were not able to couple through the inter-cage bonds formed during the 2+2 cycloaddition polymerisation reaction.