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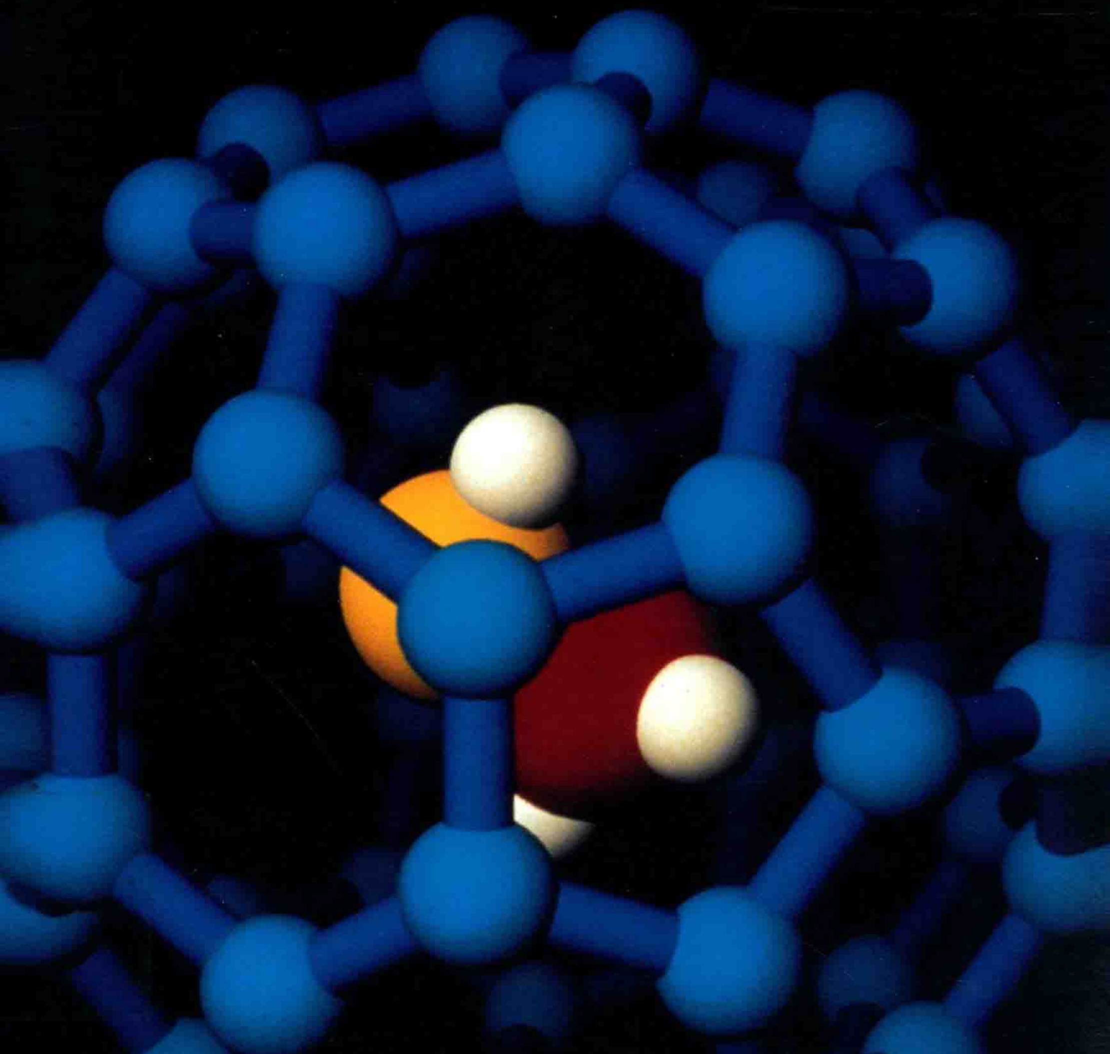
THE MOST BEAUTIFUL MOLECULE

The Discovery of the Buckyball



HUGH ALDERSEY-WILLIAMS

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THE DISCOVERY OF THE BUCKYBALL

Hugh Aldersey-Williams

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THE MOST BEAUTIFUL MOLECULE

For the chemistry masters of Highgate School in 1974 and still: Humphry Barnikel, Peter Knowles, and Andrew Szydlo, and most of all to Michael Morelle, who taught us the chemistry of Borodin, Tom Lehrer, and Flanders and Swann as well as of Lavoisier, Davy, and Mendeleev.

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CONTENTS

INTRODUCTION

The longest word in this book is also one of its most abundant. I make no apology for this, except to state the hope that I have compensated in other respects by keeping scientific jargon in check. The word is buckminsterfullerene.

As its odd name begins to imply, buckminsterfullerene, the chemical discovery that is the subject of this book, is a rather unusual substance. It has a shape that is unique in all of chemistry. Most molecules are compounds of two or more chemical elements. But a molecule of buckminsterfullerene is made up of sixty atoms of just one element – carbon. Each atom occupies an exactly equivalent site and each is joined in an exactly equivalent way to its neighbours. The chemical bonds between these atoms follow the pattern of the seams on a soccer ball that hold the leather pentagon and hexagon facets together to form the familiar inflated sphere. This spheroidal cage has the highest symmetry of any known molecule. It is, quite simply, the most beautiful molecule.

We are on intimate terms with diamond and graphite, forms of carbon which have been known for millennia. Buckminsterfullerene, or the buckyball as it was quickly nicknamed, is a third stable form; it was discovered only in 1985 and made in quantities sufficient to be able to explore its possible uses only in 1990. It was named by its discoverers after the maverick architect Richard Buckminster Fuller who popularized geodesic domes, and has since been found to be one of a family of spheroidal molecules known collectively as the fullerenes.

By virtue of its shape and symmetry, buckminsterfullerene possesses not only beauty but also novelty and likely utility. For all these qualities, buckminsterfullerene and its kin featured as the subject of nine of the ten most cited chemistry papers in 1991, as reported by an industry journal that monitors such things. In 1992, it was the subject of all ten. One paper a week appeared between 1985 and 1990. Once it was discovered how to make it in quantity, the pace accelerated to close to one a day.

Chemistry is supposed to be one of the more developed sciences. Within chemistry, carbon is the element about which we are supposed to know most. It is the element around which life is built. The remarkable thing about the discovery of buckminsterfullerene, then, is not how clever we are to have found it, but how unobservant and unimaginative we have been not to have found it sooner. The discovery is a potent reminder that science is not, as it is sometimes portrayed, on the verge of reaching a state of absolute knowledge but that after three centuries of modern chemistry we have only just begun the exploration. It highlights not how much we know, but how very little.

The story of the discovery of this unique molecule illustrates much about the way the science professions work – and occasionally fail to work – together. In its early stages, scientists – chemists, physicists, astronomers, mathematicians – collaborated fruitfully, although often without funding, driven by the excitement of a growing puzzle. Later, as pressure grew to exploit the discovery and put it to good use, the tale serves as a parable illustrating the increasing demands being placed on pure scientists to do more "relevant" work or to play a part in the development and commercial application of their new fundamental knowledge.

The discovery of buckminsterfullerene already ranks with some of the greatest moments in chemistry. As and when practical uses are found for it, its fame can only increase. The sheer beauty of the molecule has done much to revitalize chemistry teaching in schools. Equally important, it has boosted the morale of the core physical science professions with a conspicuous and inspiring success after years spent in the shadow of molecular biologists and cosmologists.

Public interest in science centres on two big questions: what is the origin of life, and what is the origin of the universe? Publishers and other popularizers of science have exploited this fascination by producing a host of books on genes and the cosmos; the physical sciences, in contrast, have been largely ignored. The startling discovery of buckminsterfullerene provides an opportunity to redress this imbalance. This tale of discovery is a celebration of the intimate world of physical science and its practitioners. It is on the face of it a self-contained tale: a molecule is born. And yet that birth is attended by the muses of many disciplines, not only the sciences but also the arts. As we shall see, this story, too, touches upon cosmology and biological science – and much else besides.

Another stereotype of "popular science" portrays research as a relentless race of one single-minded boffin against another to win the Nobel Prize. To fit this story into that mould would be to travesty a complex narrative that concerns many scientists who are humans first and – perhaps – geniuses second. (A rider to this stereotype is that the boffin is always male; this stereotype, sadly, I cannot dispel in this account.) Nevertheless, there are episodes where personal rivalry and even enmity have added fuel to the fire, and there is indeed every chance that the discoverers of buckminsterfullerene will one day be awarded the Nobel Prize.

The stereotype usually demands that serendipity play a part, an element of luck that leads to something being found that was not being sought. No one set out explicitly to discover a spheroidal sixty-atom molecule of carbon, and so to that extent we may claim that our story too has serendipity. Certainly, no one set out to overturn so completely our understanding of the physics and chemistry of carbon. Contrary, perhaps, to popular belief, it is the resolve of the modest and proper scientist *not* to seek to upset the applecart at every bump along the road. But to lay too much emphasis on serendipity is to do little justice to the skill and ingenuity of those involved, to their scientific method and to their occasionally unscientific method, and to their plain, dogged hard work. All of these qualities are of more merit than "serendipity". Serendipity, in short, is something the good scientist is prepared for, and takes advantage of.

There was no *Eureka!* moment in this story, though history may later demand that one be conjured up. Rather there were many small realizations and a creeping feeling, at first of uncertainty because things were somehow not as they should be, and then of certainty that some remarkable new phenomenon lay behind it all.

In this discovery, as in others, the scientists benefited from the occasional lucky break; but they were also hindered from time to time by an inability to break free of received wisdom and the orthodoxies of their specialisms. The story of buckminsterfullerene has its element of serendipity but also its share of these blocks. It is perhaps they which better illustrate the working of the scientific mind. The stubbornness that causes some to cling to a conventional wisdom even as evidence is presented to contradict it is not so very different from the stubbornness that advocates a radical new idea in the face of disbelief and opposition from one's peers. Both attitudes have no official place in the manual of scientific method, yet both were present in abundance in the aftermath of the 1985 discovery. The discoverers of buckminsterfullerene believed they had what they had before they could really prove it; their detractors continued to disbelieve in the face of evidence that was eventually to become overwhelming.

In parallel with this debate, evidence grew, too, for the other "fullerenes", spheroidal carbon molecules not just with sixty carbon atoms, but with seventy, seventy-six, eighty-four and other numbers. All are less perfect in their symmetry than buckminsterfullerene itself, but the structure of each suggests its own curious properties. In 1991, the canvas was broadened still further with the discovery of long "buckytubes" and then huge fullerenes, made up not of a few dozen carbon atoms, but of hundreds and thousands of atoms, yet still with the same beautiful latticework shells.

When the structure of buckminsterfullerene was finally proven to everyone's satisfaction, the prospects that such an unusual molecular architecture would have unusual properties quickly led corporations such as AT&T, Du Pont, Exxon, and IBM to invest millions of dollars in order to investigate potential applications. The most apparent characteristic is the hollowness of the cage shape, large enough to trap an atom of any element of the periodic table, and offering the prospect of fascinating modifications to the properties of the element so trapped. The exterior shell of the fullerenes is also interesting as a potential site for chemical reactions. Finally, this unique family of molecules suggests a whole microworld made up of structures of interconnecting domes and tubes with clear potential in the emerging field of nanotechnology, the skill of building machines invisible to the naked eye that will be able to perform tasks too fiddly for human hands. The ultimate goal becomes the possibility of building custom carbon architectures; joining modules of spheres, tubes and other shapes in a controlled fashion, working to a designer's blueprint.

Early conjectures as to what this new class of carbon molecules might be good for were optimistic indeed, but they were soon surpassed by reality as buckminsterfullerene derivatives quite unexpectedly showed themselves able to perform as electrical superconductors and even to exhibit biological activity against the human immunodeficiency virus that causes AIDS. Yet, as the development effort intensifies, it is important to remember that the original discovery was made in the pursuit not of commercial gain or social improvement but in the name of knowledge. At root this is a story of classic "bootleg science". No company or foundation specifically funded any search for an agent that would possess these properties. The work was done on the back of other, funded, projects and when time would allow. Yet its commercial implications are probably immense.

The truth is that there is very little correlation between the extent to which a project is funded and the importance of the resulting discoveries; or between the extent of funding and how quickly a discovery is put to the service of humankind. Because it is foolish to expect such a discovery to be put to general use very soon, I have limited the discussion of potential uses of buckminsterfullerene to the final chapters and have concentrated on the story of the discovery and its aftermath.

In the book as a whole, Chapters Two and Eight serve as tent poles across which the narrative is stretched. These chapters respectively describe the discovery in 1985 and the breakthrough in 1990 when it became possible to make useful quantities of buckminsterfullerene for the first time. These chapters are like the scherzos in a Mahler symphony, boisterous and fast-paced, the scenes of frenetic activity. Around them are more rambling, exploratory movements, the adagios of the piece. The period between 1985 and 1990 was one of frustration as scientists strove to learn more about the new molecule but could still not make enough of it to gain much headway. Chapter Three chronicles efforts to prove that buckminsterfullerene was indeed the novel molecule that it was claimed to be, efforts that were hampered by a continuing inability to produce sufficient quantities for easy experimentation. The subsequent hiatus provides us with an excuse to digress during the course of Chapters Four to Seven into topics more loosely connected with buckminsterfullerene before we rejoin the fray in Chapter Eight. Chapter Nine describes a final proof of the structure of the molecule, a proof quite as elegant and visual in its appeal as the molecule itself; Chapters Ten and Eleven conclude with a discussion of the likely uses for buckminsterfullerene and the implications of its discovery.

Chapter One sets the scene for what is possibly the greatest chemical discovery of this century. It is episodic in nature, interleaving some basic chemistry with snapshots of the obsessions of the scientists involved. Although their interests initially appear separate, they gradually converge, each person contributing an expertise that will make possible the discoveries to come. By chance, the two scientists who were principally responsible for bringing buckminsterfullerene into the world share a particular episode from their past that may have sparked their scientific creativity. It is this episode that is the subject of the following Prologue.

PROLOGUE

THE DOME OF DISCOVERY

Nineteen sixty-seven was the year of the Summer of Love. It was also Canada's centennial. To mark the anniversary, the Canadian, Quebec, and Montreal authorities threw a party for fifty million guests – the Montreal EXPO. Seventy-five countries or more spread their wares over nearly one thousand acres across two largely manmade islands in the St Lawrence river. Even as international expositions go, the scale of the event was almost beyond imagination.

It was Napoleonic France that launched the idea that a nation should periodically show off the fruits of its industry, but the first truly international exposition was held in 1851 in London. Other cities jumped on the bandwagon. Before Montreal, perhaps the most powerful image of an EXPO was of the Soviet and German pavilions facing each other starkly across the main axis of the exposition site at the Palais de Chaillot in Paris. In 1937, the fascistic architecture was an effective presage of war.

The mood was very different in 1967. Technological rationalism took the place of neoclassical bombast. Many buildings at the EXPO chose to express their nations' pride in a geometric rhetoric. The Canadian pavilion was a vast inverted pyramid. The Venezuelans constructed a group of brightly coloured cubes. Monaco favoured a forest of cylinders, while the Austrian pavilion was made up of nested tetrahedra. Over the EXPO site as a whole, the effect was as if a child had chosen to blow the entire contents of a chemical crystal-growing set in one orgy of geometric excess.

In the year that Christiaan Barnard conducted the first human heart transplant operation, belief in scientific progress was near absolute. Two years later the decade would culminate in man's landing on the moon, an event that was amply trailed in many of the exhibits in Montreal. Indeed, the strides being made in science and technology at this time were so great that, a quarter of a century later, the promoters of the Seville EXPO resorted to the same come-ons: "At EXPO'92 you'll get a foretaste of the year 2000. Space probes, satellites, high resolution TV." At Montreal, it had been the SECAM system of colour television in the French pavilion while the Soviet Union demonstrated the conditions "under which a cosmonaut will walk on the moon".

Montreal caught the spirit of the time as few other cities would have done or could have done. It drew on the wealth and confidence of the North American continent and added to it that peculiarly French combination of vision and *dirigisme* that can imagine *grands projets* and then bring them into glorious existence. The fusion brought into being an International EXPO on a scale that has not been equalled since.

In the heat of this summer, two young scientists separately made the long journey by car up from New Jersey where they had jobs with two of America's major high-tech corporations.

Rick Smalley explored the crystalline cityscape of the EXPO site in the company of his sister. With short, dark hair and blue jeans, he had the look of a typical clean-cut all-American young man. Only his unusually sharp blue eyes roving and focusing on the sights around him hinted at the single-mindedness that he brought to his research. Both physicist and chemist, he was possessed by the excitement of developments in his chosen sciences. His sister, Linda, was a teacher and his senior by just over a year. Living many hundreds of miles apart, they had not met since perhaps last Christmas or Thanksgiving. The EXPO was a good pretext for them to catch up on each other's lives.

Smalley was working for Shell Chemical Company in the quality control department of its polypropylene plant in Woodbury. A workaday job perhaps, but it was an enormous plant and the technology by which the polypropylene was made had its own excitement. It was Smalley's job to troubleshoot the temperamental production process. The plant ran twenty-four hours a day and Smalley was one of the few staff who came in at night, using the valuable quiet time to develop new analytical techniques all geared to monitoring the plastic production more effectively. Smalley was enjoying working there, but nevertheless, his routine fell rather short of his high school wish to "play at the frontiers".

Linda had flown up to Philadelphia and Rick had collected her from the airport. They were unaccustomed to upping sticks and being tourists together and this was their first visit to Canada. It was also their first time in Philadelphia. As they checked off the essential sights in the cradle of America's liberty, they began the slow process of reacquainting themselves before pressing on.

The Montreal reunion was a generally happy one. But Rick was tired from his work and the long drive, the modest hotel room they had booked was cramped and lacked air-conditioning, and under the broiling Canadian sun their conversation occasionally turned to squabbling. As they did so, a spirit of competition bubbled to the surface that had lain pretty much dormant since the two were rivals in chemistry class at high school.

On another day during the same month, Harry and Margaret Kroto, a young English couple, were pushing their infant boy along in an elaborate white pram of the kind that is now obsolete. Harry was also a scientist, a physical chemist to be exact, but with an artist's eye that was as happy in contemplation of the merits of one typeface over another as in analysing the fine structure of a molecular spectrum. Casually dressed in shirt, slacks and shades, he had been living and working in North America for nearly three years and betrayed little of that characteristic awkwardness of the English abroad.

He and his wife were relaxed and happy as they watched their son clambering over the modern plastic furniture in the cafés, although it was not without regret that they were counting down the days before they were due to leave North America for their return trip to Britain. Between touring the various national pavilions, they found time to stop and throw pebbles into one of the lakes that dotted the EXPO islands.

In the United States, Harry was working for a spell in Murray Hill at the Bell Laboratories, famous for their pioneering role in the invention of the transistor and the laser. He was using laser light to study the properties of molecules such as benzene and carbon disulphide, shining the light so that it would reveal something of how the molecules interacted with one another. It was not the sort of work that yields an easy answer for those who demand that scientific research should have an immediate commercial benefit. He was simply doing what scientists have always done, adding to the stock of knowledge about the natural world. Margaret, meanwhile, was housebound, looking after the addition to the family.

The trip to Montreal was the principal vacation of the year, and their last in North America before Harry was to return to England, drawn by an odd mix of patriotism, a wish to be closer to where the Sixties were really Swinging, and an invitation to begin an academic research career at the brand new University of Sussex.

The two couples set about touring the EXPO rather differently. The Krotos' strategy involved a map and a schedule. Their interest was as much in the cultural and creative aspects of each nation as in their demonstrations of scientific prowess. They stood in line to enter the Czechoslovakian pavilion, where Margaret was captivated by a display of contemporary glassware in cool greens and blues. Harry was more interested in the work of the film animators for which the country is famous.

The Smalleys' approach was more haphazard but ultimately more exhaustive. Rick and Linda's principal goal was to eat in as many of the pavilion restaurants as possible. They struck out at random, but by the end of their time, they had seen all the major pavilions and sampled the cuisine in many of them. Diverted momentarily from their culinary crusade, Rick was impressed by the sweeping cantilevered pavilion of the Soviet Union, and the rare glimpse it offered into a world normally hidden from view during those Cold War days. It had been the launch of the Sputnik satellite during his high school days that had stirred Rick's interest in science. Now, Rick wanted to inspect the latest in Soviet space technology.

Across a channel of water from the Soviet pavilion, linked to it by a pedestrian bridge known as the Cosmos Walk, lay the pavilion of the United States, the giant geodesic dome designed by Richard Buckminster Fuller that was the boldest architectural statement of all. The dome stood 76 metres tall. Its base was smaller than its diameter so that it appeared almost to be a complete sphere bobbing along on the surface of the Ile Sainte-Helène. Viewed from the platforms of other pavilions, the sphere seemed smooth. There was no way to gauge its size without referring to nearby trees or flagstaffs. Its alien shape and its scalelessness made it quite unlike any other building.

The outer frame of the dome was made up of steel struts linked into a repeating pattern of triangles. Six triangles came together at each point where the struts were joined, except for a number of special positions across the sphere where only five triangles met. If one were to stop focusing on the triangles, one would see the surface of the dome as a honeycomb of hexagons with, on closer examination, a few pentagonal irregularities.

Amid the ordered chaos of different nations' pavilions striving for effect, the dome had an undeniable serenity. So it was with a sense of awe that visitors pierced the tracery of tensioned steel and entered this cathedral consecrated to the theme "Creative America".

The spectacle was perhaps still more remarkable from the inside. The space was in fact quite different from that in a cathedral. The long axis of a cathedral is its nave. Here, the views stretched in all three dimensions. Light poured in from all sides of this structure without sides. There was little sense of being enclosed. Heavy platforms hovered impossibly in the vast space, setting off the feeling of weightlessness of the dome itself.

Both scientists were struck by the grandeur of the conception, although both, too, viewed it as a largely impractical one-off piece of technological bravura and not, as Fuller might have hoped, as the prototypical shape of shelter for the future. Rick Smalley was stunned by the contradiction that so transparent a structure could have such a dominating presence.

Like many Americans, he was aware of the name Buckminster Fuller, he knew what a geodesic dome was, but nothing more. Harry Kroto was more familiar with the maverick architect's work. He had seen published some of Fuller's more utopian schemes, but the Montreal dome represented the most tangible example of his principles and deserved closer inspection. Kroto negotiated his child's pram up and down the escalators and ramps that link the exhibit platforms. He drew away from the exhibit levels, and the pop-cultural clutter of Elvis Presley's guitar and paintings by Andy Warhol, to get a closer look at the structure of the dome. As he did so, hexagons dissolved into triangles and triangles into the individual components of the structure. Neither Kroto nor Smalley ever noticed the handful of pentagons insinuated among the hexagons of the gigantic orb.

In later years, both scientists' recollections of their visit to the American pavilion would become clouded. As part of his duties as an American father, Smalley made repeated visits to Disneyworld. After a time, perhaps, it was the larger dome of EPCOT that he recalled more readily. Since his student days Kroto had kept an extensive archive of magazines of the visual arts, and it was the photographs and diagrams of Fuller's EXPO pavilion in publications such as *Life*, *Graphis*, and *Paris Match* that he remembered as much as the real thing.

Lodged there by whatever means, the image of the geodesic dome that these two young scientists saw at EXPO '67 was a persistent one. It was an image that would come to assume a great importance when they first met eighteen years later.