An Arts Project Uncovering an Important Scientific Advance

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Abstract

Quite unexpectedly, a fun project to build a molecular model as a sculpture to display in our laboratory inadvertently contributed to our understanding of carbon particles at nanoscale dimensions. Heretofore attempts to explain the observations had been based on erroneous assumptions of chemico-structural behaviour. Building physical models of large Fullerene carbon cages based on Goldberg polyhedra indicted that the surface of the carbon particles would not in general be spherical and explained the structures previously observed but not understood. This seems to be a rare example of art contributing to the scientific knowledge base.

Geodesic Domes

During the period 1974-1980 a combination of chemical synthesis and spectroscopy experiments on linear carbon chain molecules, carried out with colleagues at Sussex University, led on to investigations with radioastronomers at the National Research Council of Canada which uncovered the existence of these chains in interstellar space [1]. Subsequently these unusual chains were discovered in the atmospheres of red giant carbon stars and in an experiment carried out, in 1985 with colleagues at Rice University in the US, to explain the chemical constitution of these stellar atmospheres, the serendipitous discovery was made that there existed an extremely stable carbon molecule consisting entirely of 60 carbon atoms [2]. At the moment of discovery the primary question was: What might be the chemical structure of this entity? I had walked throughout Buckminster Fuller's geodesic dome at Expo in 1967 in Montreal and its structure had made a very strong impression on me. Furthermore I had subscribed since 1958, when I started as a student at Sheffield University, to "Graphis" the iconic journal of graphic art and design, and the striking night-time image, Figure 1, in volume 132 devoted to Expo67 had become indelibly imprinted on my mind. At first sight the dome is essentially a closed spheroidal network of hexagonal struts and as the starting material for the experiment had been graphite which was known to consist of sheets of carbon atoms connected together in planar hexagonal arrays the possibility that this closed dome of hexagons might offer a clue was very persuasive in my mind. Furthermore chemical intuition persuaded us that a closed network might explain the lack of reactivity of the species, whereas an open graphene sheet should possess highly reactive carbon atoms at the open edges.

The network of struts is however quite complicated as the dome actually consists of a rather complicated double "skin" structure and furthermore the two skins are interlinked (Figure 2). A second object that was also an important key to the likely structure of the C_{60} species was the elegant cardboard stardome model shown in Figure 3a. This is a starmap which I had made for our children many years beforehand. At one point I suggested that this might also be the right structure to explain our observation but the first colleague to whom I suggested it was not at all convinced and my inclination at that moment to make an expensive transatlantic call to my home in the UK to check using his phone was unfortunately discouraged. However during a later dinner to celebrate the discovery of this provocative upstart species, whose signal towered over all the others, I described the structure from memory and pointed out to my colleagues the fact that it consisted not only of hexagons but also of pentagons.

Figure 1: *Photograph by Michel Proulx of Buckminster Fuller's Dome at the Montreal Expo in 1967 published in the magazine "Graphis" issue 132 clearly showing the basic hexagonal strut pattern. The more complex interlinking of the double skin structure is also observable but less obviously. It might be of interest to note that only the top hemisphere is actually geodesic. When I returned to Montreal after the discovery of C_{60} with a serious intrinsic interest in the structure, what I wanted to do was enter the cage through a pentagonal opening if possible. To my consternation I could not find one near ground level as I expected. I mentioned this to Ed Applewhite a former colleague of Buckminster Fuller and he pointed out that the bottom half was not actually geodesic! If the reader studies the above image carefully one can indeed see that the hexagons in the bottom half are arranged horizontally whereas in the top half they curve along geodesics. I assume that this is so the structure of the struts at ground level is horizontal, so simplifying construction problems.*

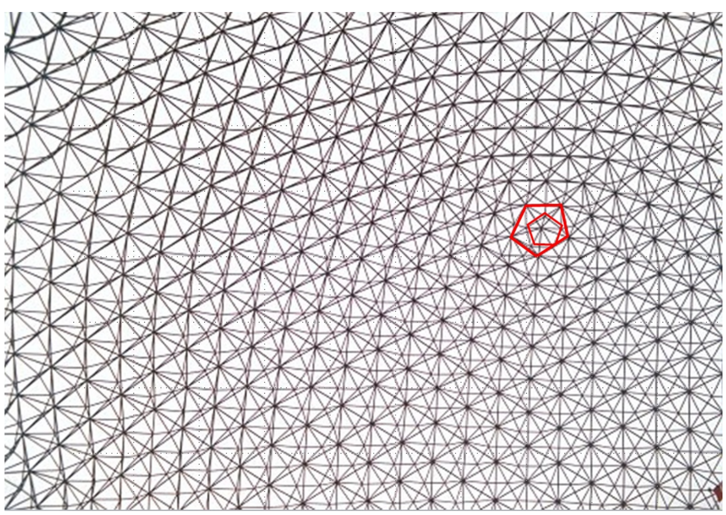
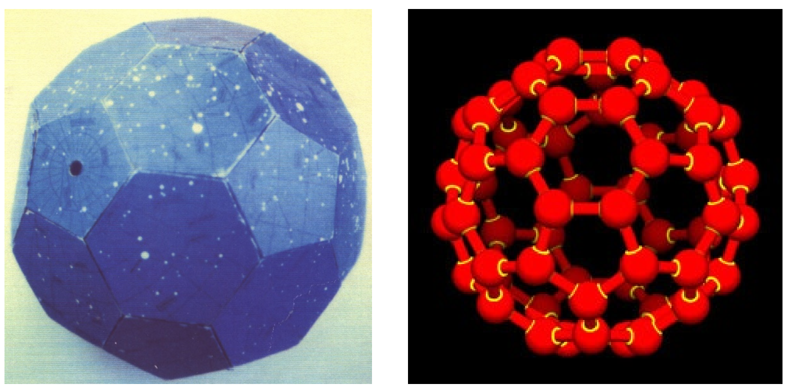


Figure 2: *The network of struts in the Expo67 Dome is quite complicated with a double skin structure in which the two skins are interlinked by complicated triangulation. I have located a pentagonal structure region in red.*

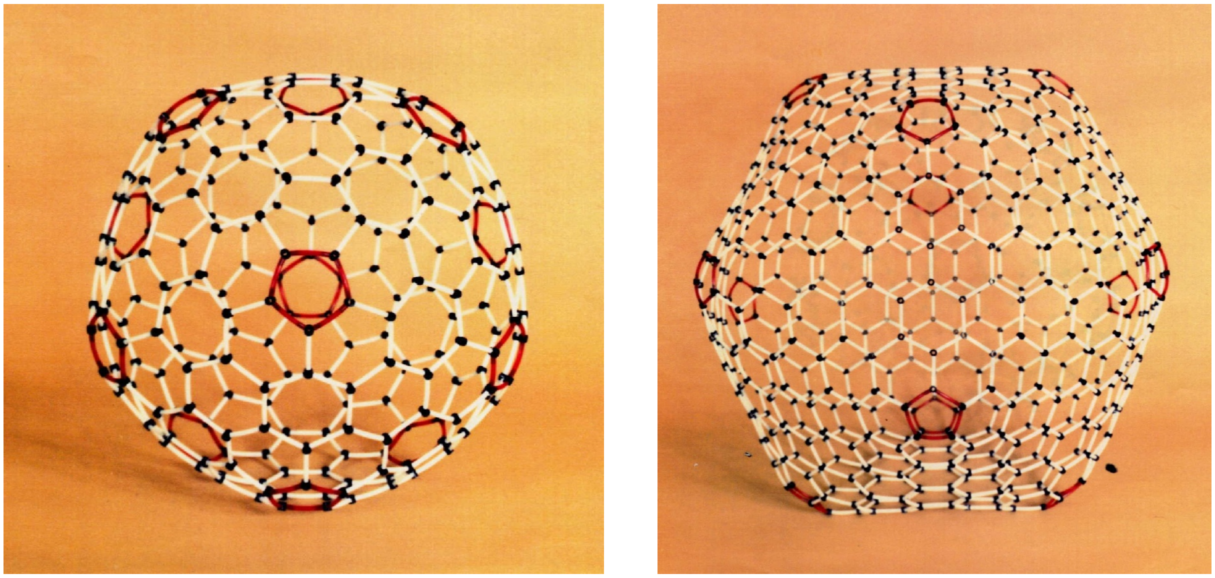
I had also earlier suggested that we withdraw a book on Buckminster Fuller's Domes from the library, which we had done. Thus the closed dome image of Figure 1 as well as in particular the pentagons of the stardome (Figure 3a) were the crucially important clues that led to the conclusion that the species had a hollow cage truncated icosahedral structure with the same pattern as a soccer ball [2, 3], (Figure 3b). As the geodesic dome had been such an important, even an iconic clue to the likely structure at least to me, I named the molecule Buckminsterfullerene [4] and later during a telephone discussion with Alex Nickon suggested that the whole family of closed carbon cages be called the Fullerenes [5]. I coined the name on the spur-of-the-moment as we deliberated over a possible title for the paper announcing our discovery. At that moment I found the fact that the -ene ending fitted perfectly from a chemical terminology perspective and that in addition the name, though a little long, scanned nicely was doubly satisfying. In the months following the publication of the discovery scores of fairly unimaginative names such as soccerene and footballene were proposed by others and I found myself defending my invention [6]. However I think it is fair to say that "Buckminsterfullerene" has turned out to be a very good choice, especially as it conveys the fact that there is an intrinsic unity between structural concepts at molecular nanoscale dimensions to the architectural dimensions of the massive structures such as that in Figure 1 that man can create on a grand physical scale. Even more intellectually satisfying from an educational perspective is the fact that it also generates in non-scientists a general awareness that delightful beauty also exists in the almost unobservable world of chemistry so helping to overcome the abstractness that is such a barrier for many to much intrinsic scientific understanding.



(a) *(b)*

Figure 3: *(a) Cardboard "Stardome" map of the sky on a truncated icosahedron. The pentagons on this object provided an important clue to the fact that structure of C_{60} has the structure shown in (b).*

Soon after the discovery of C_{60} I started to wonder about the possibility of much larger Fullerene cages with many more atoms than sixty and I thought it would be rather nice to have a model sculpture of some of these giant fullerenes hanging in our laboratory. With Ken McKay, who at the time was a PhD research student, we looked into the way to build them. Basically I thought it might be neat to build our own mini-Buckminster Fuller Dome like the one pictured in Figure 1 but preferably a "little" smaller! So I purchased molecular modelling kit to do it. I must emphasise that there was no thought at the time that this might be a research project – it was just a fun project to build a large beautiful model to display like a sculpture. The original project with Ken was thus basically "arts" inspired. The project led us first to some fascinating work by the mathematicians Goldberg and Coxeter on what are now called Goldberg polyhedra. When the models were constructed, much to my surprise they were not smoothly spherical like the Buckminster Fuller dome as I had assumed from cursory perusal of the images of all the domes I had seen. Instead models consisted of closed icosahedral monosurfaces in which the mainly hexagonal networks swept from one (red) pentagonal cusp to another (Figures 4a and b) and this led to a reappraisal of carbon nanostructures [7] and I decided to call the new large structures Giant Fullerenes [8]. Such structures had already been the subject of a most imaginative hypothetical conjecture some years earlier



(a) (b)

Figure 4: *Photographs of original molecular models of the Giant Fullerenes C_{240} (a) and C_{540} (b) [7]. The models are based on the Goldberg Polyhedra. In fact the structures might be considered sort of "double" polyhedra as the struts delineate one polyhedral surface with small faces and the lines connecting the (red) pentagons delineate a sort of icosahedral "super polyhedron". Notice that polygonal shape is more pronounced in the larger cage (b). The Giant Fullerenes are essentially icosahedral quasi-polyhedra consisting of relatively smooth surfaces which sweep between the 12 pentagonal cusps necessary for network closure.*

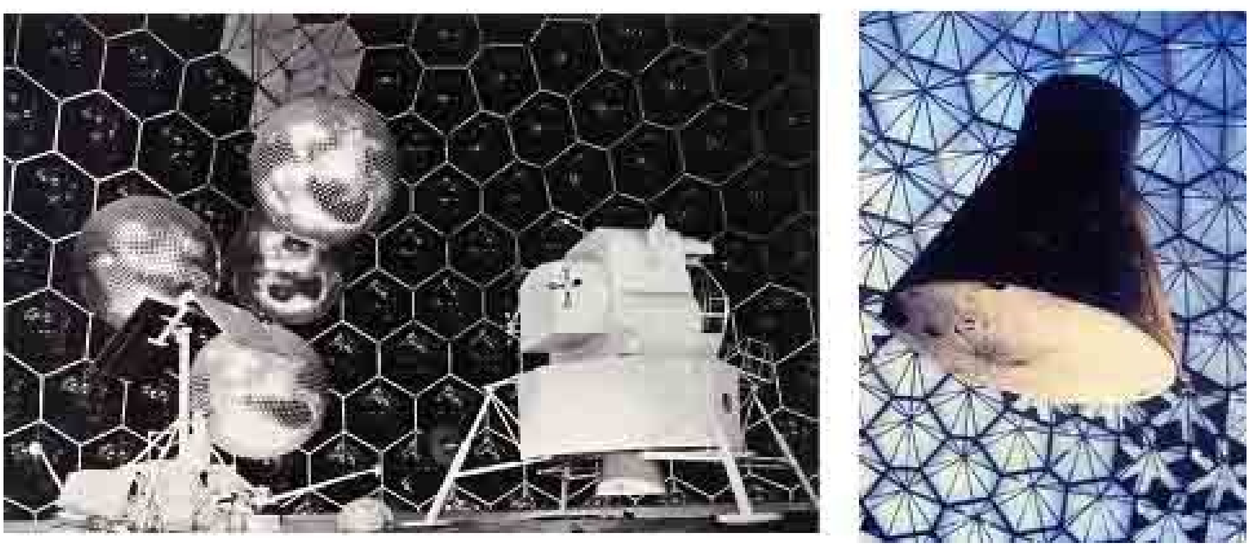


Figure 5: *Two images taken from inside the Expo 67 Dome. The left hand photograph was published in Graphis 132 and the right hand one was taken by Robin Whyman who kindly gave me a copy. By great good fortune these photographs, which are primarily of the Eagle Moon Lander replica and the first US space capsule, both fortunately show pentagons. Particularly interesting from the science/art point of view is the asymmetry of the hexagons which abut the pentagons. This distortion is necessary to produce the near spheroidal structure of the Expo67 Dome.*

in 1966 by David Jones and published in the New Scientist under the pseudonym Daedalus [10]. Indeed the equally imaginative and prescient conjecture that C_{60} itself might be stable had also been published by Eiji Osawa in 1970 [10].

When Ken brought the model of C_{540} he had constructed into my office I remember being immediately perplexed as to why it was not smoothly spheroidal as I had expected. Then we returned to study images of Fuller's domes and fortunately I had a couple of photographs taken from inside the Expo 67 dome, both of which, even more fortuitously, showed the regions in the vicinity of pentagons. Study of these images indicated that although the majority of the hexagons was symmetric, those in the immediate neighbourhood of the pentagons were quite distorted as can be seen in Figure 5.

Then we realised that I (and apparently everyone else) had overlooked something that had been under our noses in the literature for years. I had studied transmission electron microscope images of spheroidal carbon particles several times in the past and only now realised what I must have been looking at. Several years earlier high resolution electron microscope images of onion-like structures had been published by Iijima [12]. A typical example of one of these structures is shown in Figure 6, which is one of the elegant images obtained by Daniel Ugarte. The transmission electron microscope yields an image that can be considered a sort of cross-section of the spheroidal particle that consists of concentric more-or-less spheroidal onion-like shells revealing the inner structure in much the same way that cutting horizontally through a tree trunk reveals tree rings. What I realised was that I and other had missed the fact that the rings were not quite smoothly circular but possessed subtle curvature variations which betrayed the fact that they were actually quasi-icosahedral shells with shapes similar to our Giant Fullerene models. It then became clear that the observed structures were the result of entirely sp^2 trigonal bonding resulting in a closed-cage network in which the equivalent of 12 pentagonal disclinations are dispersed among the myriads of hexagonally arrayed carbon atoms. Indeed the tetrahedral sp^3 bonding that had previously been invoked to overcome the topological requirements of Euler' Law is quite unnecessary.

Figure 6: *High resolution transmission electron microscope image of an onion-like spheroidal carbon particle. Flattening of the shells is most obvious in the outer arcs between 8 o'clock and 11 o'clock. Image by Daniel Ugarte.*

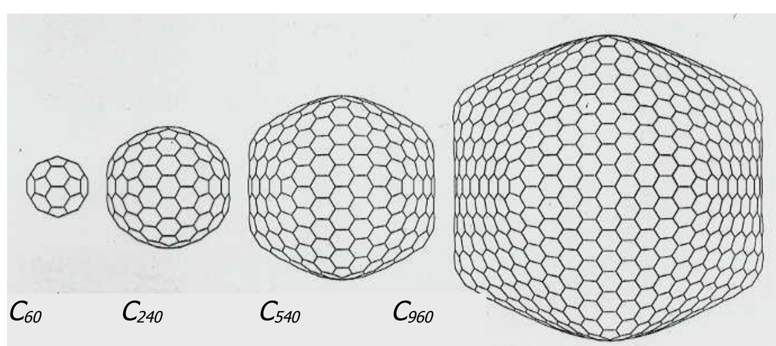


Figure 7: *Set of Fullerenes of gradually increasing size. Note that as the size of the Fullerenes increase, the quasi-polyhedral shape emerges and becomes more obvious.*

I realised I had not seen what was actually there but what I had assumed was there and to confirm the new perspective and obtain quantitative confirmation of this conjecture Ken wrote computer programmes [7] to create a set of Giant Fullerenes of ever increasing size (Figure 7).

Several cages were then placed one inside the other in onion-like configurations and the electron microscope images computer simulated [12]. In a transmission electron microscope (TEM) a beam of electrons is passed through an object and if the beam encounters an array of atoms which possess some phase relation, as they do when the electrons pass along a channel in which a graphite wall lies, then the electrons may be scattered and a dark line appears in the resulting diffraction pattern as shown in Figures 8 a and b. One then observes what is effectively a cross-section of the particle and nested Fullerene structures tend to show polygonal rings with something between 6-fold and 10-fold symmetry. Of course perfect icosahedral symmetry is unlikely but flattening should be, and is, commonly observed, Figure 6 and Figure 9.

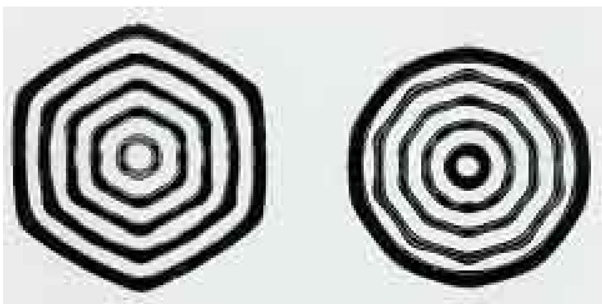


Figure 8: *Simulated high-resolution electron microscope images of a carbon particles consisting of 5 concentric Fullerene cages seen along two different axes; a) The left hand image shows 6-fold symmetry whereas b) the right hand image shows 10-fold symmetry.*

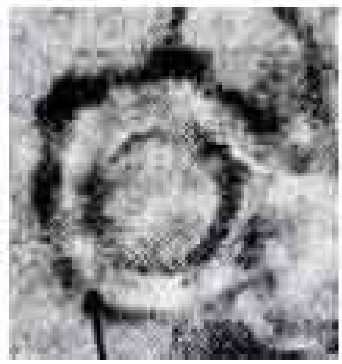


Figure 9: *An actual high resolution electron microscope image of a carbon particle consisting of two shells. The approximately hexagonal shape of the outer shell is clear and is consistent with the simulation shown in Figure 8a. (Image from Mordkovich and Endo.)*

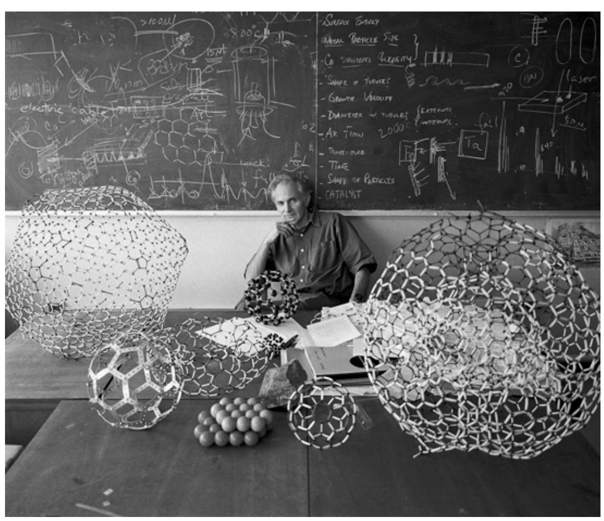


Figure 10: *The Fullerene menagerie at the University of Sussex's NanoScience and NanoTechnology Centre with a somewhat pensive zoo-keeper. Photograph by Ann Katrin Purkiss, Image courtesy of the Wellcome Trust Image Library.*

The upshot of this project is that we ended up with a room full of molecular models of giant fullerenes (Figure 10).

Particularly satisfying is the fact that the structure has stimulated numerous educational science projects in schools. One such project is shown in Figure 11 in which a large Buckyball is being constructed by a group of high school students in Angmering, West Sussex UK. As far as I am concerned this image gives me intense personal satisfaction as I have never seen a more wonderful example of the value of marrying Science, Art, Architecture, Engineering and Mathematics in an intrinsically hands-on educational teamwork project.

Finally, most satisfying personally is the fact that in front of the main entrance to Sheffield University's Kroto Research Institute in the UK stands the Giant Fullerene metal sculpture I designed, shown in Figure 12.

Figure 11: *Photograph of children at a school in Angmering UK constructing a large 9 foot diameter model of C_{60} made out of strips of plastic.*

Figure 12: *Giant Fullerene sculpture, 5' in diameter, in front of the Sheffield University's Kroto Research Institute, glistening under floodlight at night.*

Conclusion

In this paper an account is given of a project which was originally initiated to satisfy an aesthetic creative impulse to build a 3-dimensional sculpture based on a chemical structural recipe. In the event the resulting model turned out to have an unexpected subtle shape with structural characteristics which led to an explanation of some important nanoscale structural observations that had been made some years previously and mistakenly explained. This appears to be a rather rare example of the way a creative project in the arts resulted in an important advance in science.

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References

[1] *Semistable Molecules in the Laboratory and in Space,* Royal Society of Chemistry Tilden Lecture; H W Kroto, Chem. Soc. Revs., 11, 435-491 (1982).

[2] *C60: Buckminsterfullerene,* H W Kroto, J R Heath, S C O'Brien, R F Curl and R E Smalley, Nature, **318** (No.6042), 162-163, (1985).

[3] *Space, stars, C_{60} and Soot*, H.W. Kroto, *Science*, **242**, 1139-1145 (1988); *Probing C_{60}*, R F Curl and R E Smalley, Science **242** 1017-1022 (1988); *C_{60}: Buckminsterfullerene, the celestial sphere that fell to earth*; H.W. Kroto, *Angew. Chem. Internat. Edit. Engl.*, **31**, 111-129 (1992); *Symmetry, space, stars and C_{60},* H W Kroto, Angew. Chem. Int. Ed. Engl., **36**, 1578 (1997) and Rev. Mod Phys, **69**, 703 (1997); *Dawn of the fullerenes,* R F. Curl. Rev Mod Phys, **69** 691-702 (*1997*); *Discovering the Fullerenes,* R E Smalley, Rev Mod Phys, **69** 723-730 (1997); *C_{60} Buckminsterfullerene,* H W Kroto, A W Allaf and S P Balm, Chem. Revs., **91**, 1213-1235 (1991).

[4] *The Naming of Buckminsterfullerene,* E.J. Applewhite, Chemical Intelligencer, ed. I Hargittai July 1995 Vol 1 No3 Springer Verlag. (http://www.4dsolutions.net/synergetica/eja1.html)

[5] *Organic Chemistry - The Name Game Modern Coined Terms and their Origins,* A Nickon and E F Silversmith (Pergamon New York 1987).

[6] *What's in a name?*, H W Kroto, Nature (Correspondence) **322** 766 (1986)

[7] *The Formation of Quasi-icosahedral Spiral Shell Carbon Particles,* H W Kroto and K G McKay, Nature, **331**, 328-331 (1988).

[8] *Fullerene cage clusters. The key to the structure of solid carbon*, H.W. Kroto, J. Chem. Soc., Faraday Trans., **86**, 2465-2468 (1990).

[9] *Daedalus Column* D E H Jones, New Scientist (3 Nov 1966) **245** 118-119; *The Inventions of Daedalus*, D E H Jones, Freeman Oxford 1982).

[10] *Superaromaticity,* E Osawa, Kagaku, Kyoto, **25** 854–863 (1970); *Aromaticity,* Z Yoshida and E Osawa (Kagakudojin Kyoto 1971 in Japanese).

[11] *Direct observation of the tetrahedral bonding in graphitized carbon black by high resolution electron microscopy,* Iijima, S. (1980b) J. Cryst. Growth, **50,** *675*–683.

[12] *Simulated transmission electron microscope images and characterisation of the Icospiral,* K.G. McKay, H.W. Kroto and D.J. Wales, J. Chem. Soc. Faraday Trans., **88**, 2815-2821 (1992).