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Molecular Modeling of Fullerenes with Beads

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Supporting Information

ABSTRACT: Physical molecular models are useful research and educational tools to demonstrate the bonding between atoms and to highlight the three-dimensional nature of chemical structures. Inexpensive three-dimensional physical models of arbitrary fullerenes can be accurately constructed through mathematical beading with the so-called right-angle weave stitch.

KEYWORDS: *First-Year Undergraduate/General, General Public, High School/Introductory Chemistry, Demonstrations, Public Understanding/Outreach, Analogies/Transfer, Hands-On Learning/Manipulatives, Group Theory/Symmetry, Molecular Modeling, VSEPR Theory*

Spherical polyhedra excite the imagination not only of mathematicians, engineers, and architects, but also of biologists and chemists. "Molecular modelling is a constitutive, yet overlooked, element of the practice of chemistry."[1] A case in point is C_{60} or Buckyball, where paper models played a pivotal role in elucidating the truncated icosahedral shape of C_{60}, for which Kroto, Curl, and Smalley were awarded the 1996 Nobel Prize in Chemistry.[2] Unfortunately, some molecular structures, including fullerenes, are inaccessible with standard molecular modeling kits due, in part, to the large number of atoms involved.

Herein, a simple method to construct molecular models for arbitrary fullerenes using beads is described.[3−6] In a short amount of time, students of all ages can create a fullerene museum on their desk. A bead model of C_{60} constructed from 90 beads and a single nylon fishing thread is shown in Figure 1A. In an over-simplified view, bead models represent the Gillespie's electron-pair domain model[7] for trivalent systems where each bead represents the electron density of a carbon−carbon bond in the fullerene. Owing to the similarity between microscopic valence shell electron pair repulsion and macroscopic mechanical hard-sphere interactions in the trivalent beaded models, the shape of a bead model is similar to the true molecular structure of the corresponding fullerene.

Fullerene beadworking uses a standard oriental weaving technique known as the figure-eight stitch or the Hachinoji−Ami stitch in Japanese beading. This technique, closely related to the right-angle weave in North America, is popular in oriental countries for making three-dimensional beadworks. This technique can be used to make rings, necklaces, bracelets, and now fullerenes! Any kind of beads can be used to construct beaded fullerenes. Spherical beads are ideal for making robust beadworks of all sizes, whereas tubular beads can be used to make skeletal models reminiscent of Dreiding stereomodels, where atoms are represented by the point of intersection of the beads. In both cases, two ends of nylon thread (i.e., fishing line) are used and cross in opposite directions through the beads in a figure-eight pattern as shown in Figure 1B.

To illustrate the use of the figure-eight stitch for the construction of fullerenes, begin with the simplest carbon cage, C_{20}, which is simply a dodecahedron consisting of 20 vertices, 30 edges, and 12 pentagonal faces. Because the beads represent the bonds in fullerenes, 30 beads are needed to make a beaded dodecahedron. About 100 cm of nylon thread is also required if 1 cm beads are chosen. Start by threading 5 beads in the center of the beading thread. Pass one end of the thread through the last bead at the other end of the thread to give a five-membered ring of beads with both ends crossed through one bead as shown in Figure 1B. Thread four beads on the left-hand thread and pass the right-hand thread through the last bead on the left thread to form the second five-membered ring of beads. One

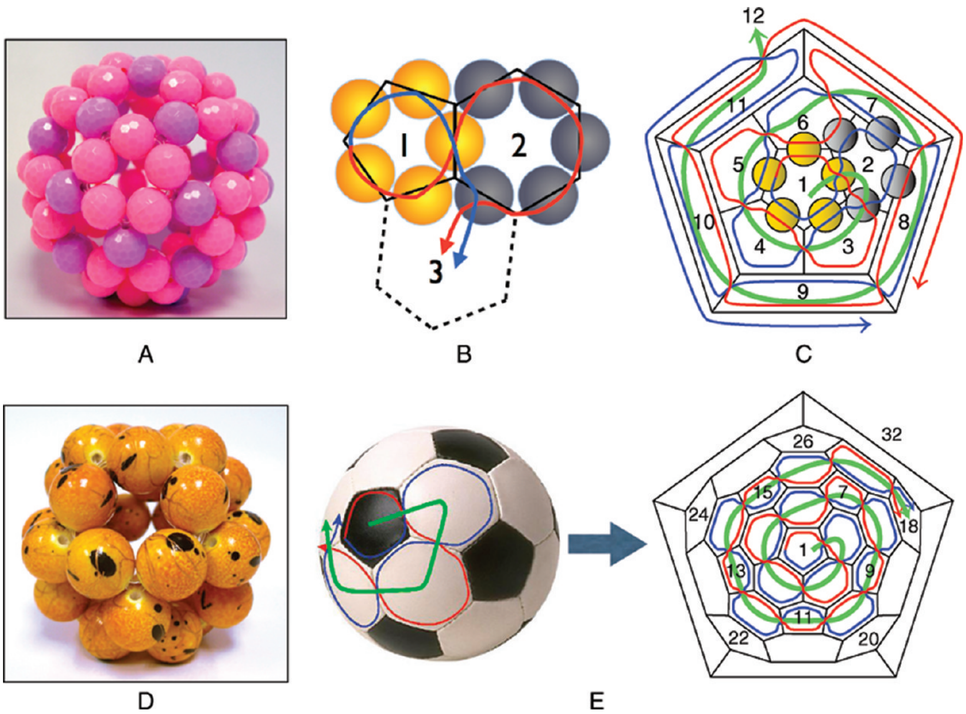

Figure 1. (A) Bead model for C_{60}, (B) figure-eight stitch, (C) the planar diagram for C_{20}, (D) bead model for C_{20}, and (E) the planar diagram for C_{60}.

then follows the planar diagram for C_{20} (Figure 1C) to make the remaining 10 pentagons. To make your C_{20} beadwork firm, pull the thread tight every time you finish a ring. When finished threading the last five-membered ring, the remaining thread can be weaved into the eyes of neighboring beads to make the resulting bead model more secure. The more you weave back, the stronger your bead model becomes. Finally, you can cut the remaining thread off to obtain your free model (Figure 1D).

The requirement for 12 pentagonal faces in C_{20} is not a coincidence. Euler developed the polyhedral formula, $v - e + f = K$, in 1750, where v, e, and f are the number of vertices, edges, and faces of a polyhedron, respectively, and K is the Euler characteristic and is related to the number of holes, g (for genus), in the polyhedron by the formula, $K = 2 - 2g$. For simple cage-like polyhedral fullerenes (without holes; $g = 0$, so $K = 2$), C_v, made up of only hexagons and pentagons, the number of pentagonal faces is always 12, the number of hexagonal faces is $(v - 20)/2$, and the number of edges (or beads) is $(v \times 3)/2$.[8,9] To make any fullerene, weave face by face with beads using the figure-eight stitch according to its pentagon spiral code.[10] For instance, the spiral code for C_{60}, [1 7 9 11 13 15 18 20 22 24 26 32], gives the position of 12 pentagons in the spiral sequence of 12 pentagons and 20 hexagons (Figure 1E). The direction of weaving follows a clockwise spiral direction, which starts from the central core pentagon and then moves around the five-fold symmetry axis outward toward the last pentagon, corresponding to the infinite area outside the planar diagram. A more detailed procedure for constructing a beaded C_{60} model is provided in the Supporting Information and condensed instructions in a tabular format are provided in ref 4. With minimal practice, a beaded model of C_{60} can be made in 30 min. By using these prescribed spiral codes, one can create realistic representations of almost any size of cage-like fullerene (Figure 2). The icosahedral fullerenes in Figure 2 clearly highlight Euler's requirement for 12 pentagons

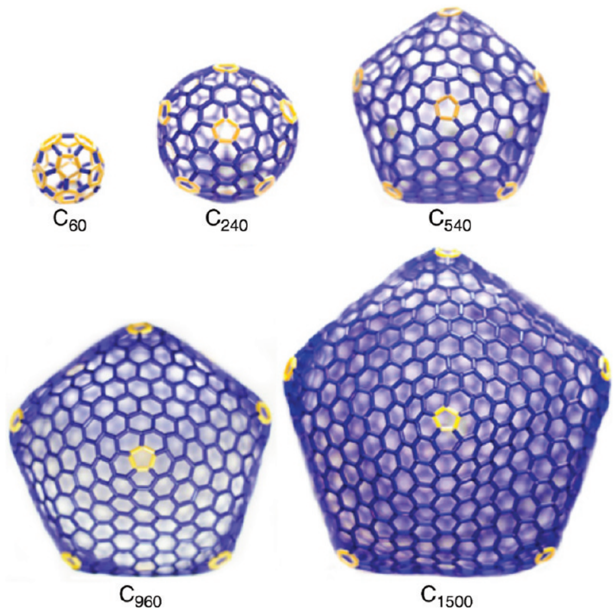

Figure 2. Bead models of five fullerenes with icosahedral symmetry (C_{60}, C_{240}, C_{540}, C_{960}, and C_{1500}).

to close a polyhedron. Unsurprisingly, the absence of pentagons leads to a flexible graphene sheet that can be easily rolled up to highlight the different orientation of armchair and zigzag carbon nanotubes (Figure 3).[11]

Finally, in addition to the cage-like fullerenes ($g = 0$), beads can also be used to construct other more complicated graphitic structures such as toroidal carbon nanotubes ($g = 1$; Figure 4),[12] high-genus fullerenes, and so forth.[5,6,13] According to our experience, beads can be used to construct robust physical models of simple and complicated carbon nanostructures that are otherwise inaccessible.

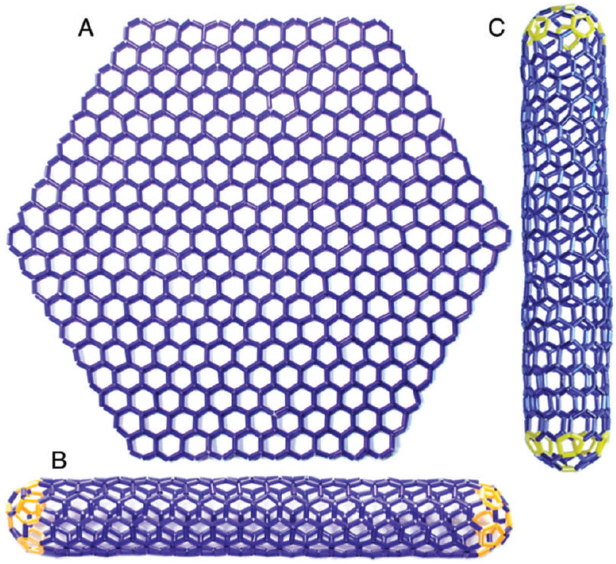

Figure 3. Bead models of a (A) sheet of graphene, (B) a C_{60}-capped armchair nanotube, and (C) a C_{80}-capped zigzag nanotube.

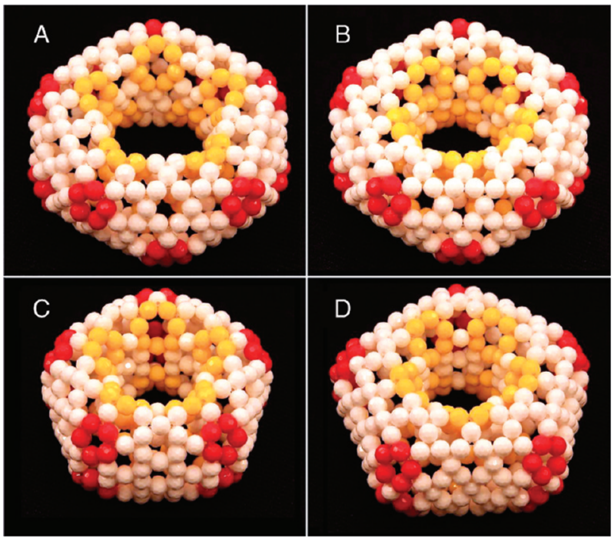

Figure 4. Bead models of carbon nanotubes: (A) D_{5d}, symmetric C_{240} with eclipsed nonhexagons; (B) D_{5d}, symmetric C_{240} with staggered nonhexagons; (C) D_{5h}, symmetric C_{210} with eclipsed nonhexagons; and (D) D_{5h}, symmetric C_{240} with staggered nonhexagons.[11].

■ ASSOCIATED CONTENT

Supporting Information

Instructions for creating the models. This material is available via the Internet at http://pubs.acs.org.

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