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A C_{60} FULLERENE MODEL AND SEPAK TAKRAW BALLS

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Abstract: In the first half of this paper, we solve the problem of how many different sepak takraw ball patterns can be made from six polypropylene bands of different colors. An important point here is chirality. In the paper's second half, we adopt a mathematical point of view to discuss the positions of the 60 carbon atoms and single and double bonds in C_{60} fullerene, which has the shape of a truncated icosahedron.

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1. Two Weaving Patterns

In October 2013, I received an email from Professor Robert L. Whetten in the United States, which contained an attached PDF file with an article about metal halides and a note thanking me for my paper that he had cited [1]. Because I'm not a chemist, I thought this email might have been sent by mistake.

Going through the attached article, the photograph in Fig. 4(d) caught my eye: sepak takraw balls on a Texas lawn. I recalled the article I had written about sepak takraw balls [3] and wondered what the relation to the chemical

compounds might be. The article used a sepak takraw ball as a model of the structure of a chemical compound with the formula I-$Au_{144}Cl_{60}$ containing 144 gold atoms and 60 chlorine atoms.

The photograph showed three balls in a row. In the center was a larger plastic ball, like the kind used for competitions, and on either side of it was a smaller ball made of paper bands in six different colors. I wondered why there were two smaller balls when one would have been enough. Looking closely at the paper balls, I noticed subtle differences. Although the order of the six colors was the same, the overlapping (weaving) of the bands was different (this point is explained later). In chemistry, this is called chirality.

Presumably, the metal halide I-$Au_{144}Cl_{60}$ has a structure analogous to that of C_{60} fullerene. Around that time, the editorial committee of a certain mathematical journal had asked me to submit a problem, and I was under a lot of pressure to prepare one. The email from Texas gave me the hint I needed to think up a rather interesting problem, which I submitted to the journal [4].

2. How Many Sepak Takraw Ball Patterns can be Prepared Using Bands of Six Different Colors?

[Problem definition]

A sepak takraw ball can be made with six polypropylene (PP) bands, which are used for packing. How many different sepak takraw ball patterns can be made if each of these bands has a different color (Fig. 1)?

(Note) Sepak takraw is a ball game from Southeast Asia that uses a ball shaped as a truncated icosahedron with 32 faces. Each three bands are in a three-way deadlock configuration and do not come loose, and each band follows a great circle path. The hollow regions are regular pentagons.

Figure 1: A sepak takraw ball (six bands of different colors)

[Solution and discussion]

Answers were received from 45 respondents aged between 20 and 80 years: 14 people (31%) answered 12 patterns, 20 people (45%) answered 24 patterns, 6 people (13%) answered 48 patterns, and 5 people (11%) gave some different answer. This resembled a three-choice problem with 12, 24, and 48 patterns as the possible answers, where 24 is the correct answer. People who answered 12 patterns did not realize that there are two weaving patterns (chirality), and those who answered 48 patterns did not realize that the order of colors at the north and south poles is reversed. There were no respondents who answered 24 patterns by accident without realizing either of the above points.

Since there are six bands, I thought that the number of patterns might be

$$6! = 720,$$

but when I solved the problem, I was left with the feeling that the number of actual patterns was unusually small. Also, it was pointed out that the overlapping (weaving) pattern was the reverse of that of the competition sepak takraw ball shown in the problem definition, but both types of balls were regarded as valid sepak takraw balls, regardless of the overlapping pattern.

Let me explain the method for making sepak takraw balls since it is important to solving the problem. Take six PP bands 15 mm in width and 56 cm in length (twice the circumference of the ball). The sepak takraw ball can be constructed in a natural manner by observing the following two rules [3]:

(1) Each three bands are in a three-way deadlock configuration
(2) Each five bands describe a regular pentagon

There are 12 regular pentagons and 20 regular hexagons forming a truncated icosahedron, similarly to a soccer ball. In Figure 2, the hollow section (in black) is a regular pentagon, and the area formed by drawing dotted across the regions where each two bands overlap is a regular hexagon. Readers who have yet to make one of these balls should by all means give it a try. The process from the configuration in Fig. 2 to a complete sepak takraw ball closely resembles the process of forming a C_{60} fullerene from corannulene ($C_{20}H_{10}$) (discussed later).

Sepak takraw balls can be constructed from six PP bands, in which case the bands are related to the six great circles of a regular icosahedron (Fig. 3). A regular icosahedron is constructed from 20 equilateral triangles, and has 20 faces (F), 30 edges (E), and 12 vertices (V). The Euler characteristic is
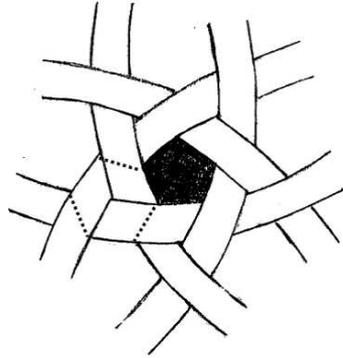
$$F - E + V = 20 - 30 + 12 = 2.$$

Figure 2: The hollow sections are regular pentagons, and regular hexagons are obtained by drawing dotted lines across the bands

Bisecting a regular icosahedron with a plane perpendicular to an axis forms a great circle in the cross-sectional plane, and there are six such great circles [5]. A sepak takraw ball can be constructed by placing PP bands along these great circles (Fig. 1).
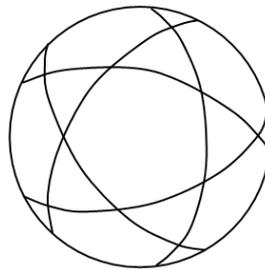

Figure 3: The six great circles of the icosahedron [5].

As explained above, a sepak takraw ball contains 12 regular pentagons. We will use the terms equator, north pole and south pole by analogy with the Earth, and we label the bands A to F.

Let us focus on one regular pentagon (north pole) and label it P. The five edges of P are composed of five different colors, and due to symmetry, the sixth differently colored band follows the great circle (equator) that is perpendicular to the line passing through the center of P and the center of the sphere. We fix the color of this sixth band as A.

Using cyclic permutation, the number of combinations of the remaining five bands B-F is

$$(5 - 1)! = 4! = 24.$$

Here, the order of colors of the bands describing P (north pole) are taken as B, C, D, E, and F in the counterclockwise direction. For the regular pentagon lying exactly opposite P (south pole), the color order is reversed as the pentagon is flipped upside down. This becomes obvious from the relation between the positions of the six great circles of the regular icosahedron in Fig. 3. Therefore, in the 24 patterns we obtained, each distribution and its reverse are counted twice, and dividing by 2, we obtain

$$24 \div 2 = 12 \; patterns.$$
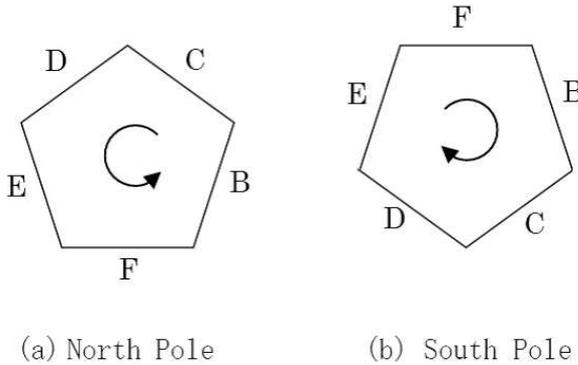

(a) North Pole   (b) South Pole

Figure 4: The color order is reverse on the north and south poles

Next, focusing on the deadlock configuration of the bands, we can obtain a right-hand (clockwise) or a left-hand (counterclockwise) pattern (Fig. 5 (a) and (b)) depending on whether the bands are woven by overlapping them from above or below. Therefore, doubling the above result, we obtain

$$12 \times 2 = 24 \; patterns.$$

which is the final result. Patterns in (a) and (b) are in a chiral relation. Specifically, they are enantiomers, which are non-superimposable mirror images.

With the above discussion in mind, the following are actual sepak takraw balls. There are two types of balls for each color order because there are two
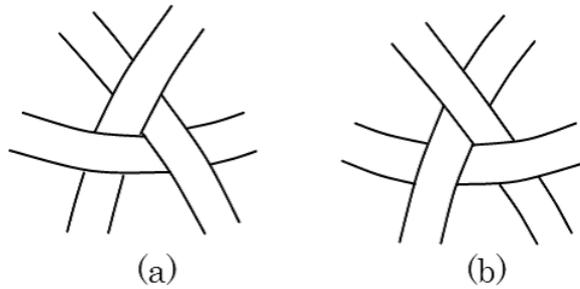
Figure 5: Two types of three-way deadlock configurations

ways to overlap the bands (Fig. 6). Furthermore, Fig. 7 shows all 12 ball patterns where the overlapping pattern is fixed and only the color combinations are permutated.

Figure 6: Two types of overlapping

Let us consider how the truncated icosahedron is related to soccer balls and sepak takraw balls. The truncated icosahedron is a regular icosahedron with the vertices cut off, and consists of 12 regular pentagons and 20 regular hexagons, for a total of 32 faces. It has 60 vertices (Fig. 8 (a)). Expanding the regular pentagonal and hexagonal faces in the radial direction gives the soccer ball (Fig. 8 (b)), in which case the coordinates of the vertices do not change. Weaving bands following the six great circles of the regular icosahedron gives the sepak takraw ball, where the vertices of the hollow pentagonal sections correspond to the vertices of a truncated icosahedron (Fig. 8 (c)). It should be noted that the positions of the vertices of the pentagons on balls prepared from PP bands are more accurate than those of balls used in competitions (Fig. 1).

Figure 7: Twelve color patterns

The soccer ball is often given as an example of the molecular model of a C_{60} fullerene, but I think that the sepak takraw ball is more suitable for representing a truncated icosahedron with a familiar object. A sepak takraw ball can be easily constructed from six PP bands, and its interior can be easily observed because the pentagons are hollow. If a metal atom is embedded into a truncated icosahedron, it resembles a metal atom enclosed in fullerene. The sepak takraw ball has many excellent properties, for example, the three-way deadlock coupling (weaving) makes the ball sturdier, and the size (diameter) of the ball can be determined solely by the width of the bands [3].

Sometimes the enchanting nature of the sepak takraw ball can make the paths followed by the bands seem like electron orbitals. The 120 free electrons ($12 \times 5 + 30 \times 2 = 120$) in the outermost shell of the C_{60} fullerene may be expected to move along such orbits, but there is an inconsistency in this hypothesis.

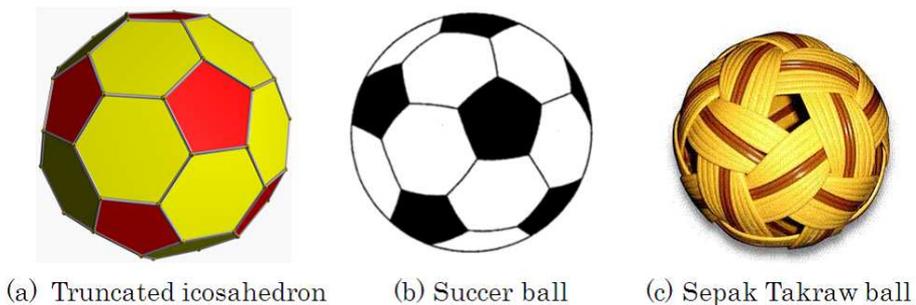(a) Truncated icosahedron   (b) Succer ball   (c) Sepak Takraw ball

Figure 8: The truncated icosahedron group

The sepak takraw ball also has the following properties. The PP bands overlap at a total of 30 locations. If these locations are marked with double lines as in Fig. 9, it forms a model of the carbon bonds in a C_{60} fullerene (the Kekulé structure with single and double bonds) (Fig. 12 (a)).

3. Molecular Model of the C_{60} Fullerene

In 1985, Kroto et al. discovered a new form of carbon: a C_{60} molecule shaped like a soccer ball [6]. This molecule was named buckminsterfullerene after the architect Buckminster Fuller, whose geodesic domes offered a clue to the structure of C_{60} fullerene. In 1996, H. W. Kroto, R. F. Curl, and R. E. Smalley received the Nobel Prize in Chemistry. However, the possibility of the existence of such molecules was theoretically predicted in 1970 by E. Osawa [10].

Figure 9: Double lines drawn across the bands at the locations where two bands overlap

Since the announcement of its discovery in 1985, I have been interested in the distribution of the 60 carbon atoms in C$_{60}$ fullerene. This is because it has solved five puzzles related to biological evolution in my research. Thinking about why there are so many flowers with 5 petals, why the starfish has 5 arms, and why humans have 5 fingers on each hand, the number 5 seems to be lurking everywhere in nature. I have used truncated icosahedra to model the 32-cell stage during cleavage in developmental biology as well as the cell distribution at the shoot apex during flower bud formation [2].

The cell distribution at the 32-cell stage during cleavage in early embryogenesis resembles the structure of C$_{60}$ fullerene. Both structures are related to a truncated icosahedron. The truncated icosahedron has 60 vertices, 32 faces, and 90 edges, and placing a carbon atom on each of those 60 vertices gives a C$_{60}$ fullerene, whereas placing an embryonic cell in each of the 32 faces gives the 32-cell stage of the starfish egg.

While the truncated icosahedron is fairly close to a sphere, the locations of the 60 vertices are not completely uniform. The regular pentagons are smaller than the regular hexagons. If they were completely uniform, would the regular pentagons become slightly larger and the regular hexagons or slightly smaller? This is a rather interesting point. Also, there are problems particular to the chemistry of the C$_{60}$ fullerene, such as electrons in the outermost shell and valence. The reality is that C$_{60}$ cannot be treated in the same way as the distribution of cells in biology.

While searching for a way to obtain a better understanding of the molecular structure of C$_{60}$ fullerene, the Professor R. L. Whetten, mentioned in the introduction, told me about Jmol, an open-source program for viewing the 3D chemical structures. Installing Jmol on my PC was not that difficult. Then, I used C$_{60}$ data available via the Internet (file name: C60.xyz) to display the structure of C$_{60}$ (Fig. 10). Jmol allows the user to rotate the C$_{60}$ molecule and

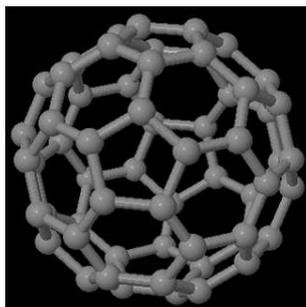to get an idea about its three-dimensional structure.

Figure 10: C_{60} displayed in Jmol

I shifted my attention to the data in the C60.xyz file, which consisted of a total of 62 lines. The first line was '60', which probably indicated the number of atoms. The second line was probably a title line, which, as I found out, could be left blank. Lines 3 to 62 had the same format, with 'C' in the first column followed by three numbers separated by blank spaces. The initial 'C' most probably stands for a carbon atom, and the three numbers most likely represent x, y, and z coordinates. The file extension was xyz, and the full file name was C60.xyz. The following is an excerpt from the file.

```
(Jmol data example C60.xyz)
60
Buckminsterfullerene C60 model
C    -1.415441    3.015027    -1.167954
C     2.583693    2.292084    -0.721147
C     0.721155    -2.583700    2.292090
cccccccccccccccccccc
```

Is it OK to have just the coordinates of the carbon atoms? In general, in order to display a three-dimensional image, it is necessary to have not only the coordinates of the vertices, but also information about the structure of the edges of each face as well as information about the points of each edge. I thought it was somewhat strange that it is unnecessary to have the numbers of carbon atoms constituting five-membered and six-membered rings and information about which carbons are connected. And yet, the Jmol system calculated the information about edges and faces just from the 60 coordinates.

Using several Jmol files (C60.xyz) downloaded from the Internet, I investigated the relation between the positions of the carbons when displaying the molecular model. I prepared Fig. 11 to help with understanding the three-dimensional image. In (a), the gray and white areas indicate five-membered and six-membered rings, and the black dots are carbons. In (b), the carbons are numbered, and it is easier to understand the relations between the bonds.
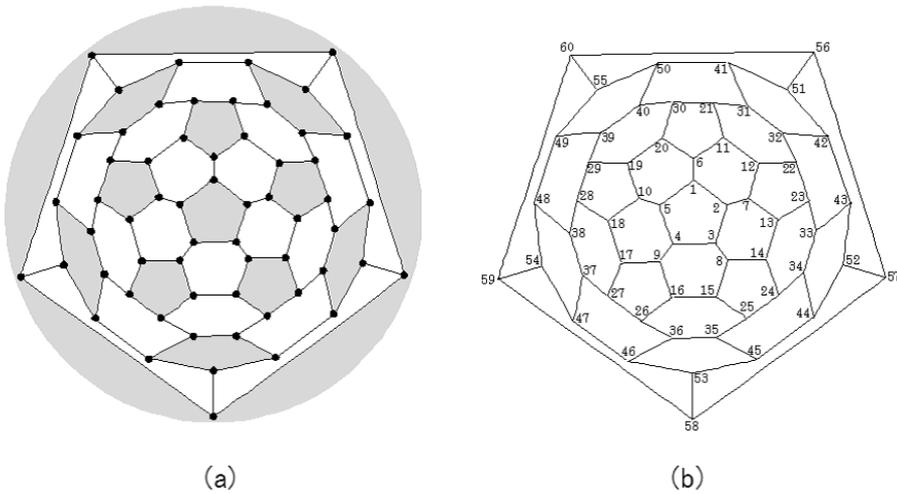

(a)   (b)

Figure 11: Network diagram

The coordinates in the C60.xyz file are taken as

$$\{(C_i(x), C_i(y), C_i(z)), i = 1, \cdots, 60\}$$

Next, $O(x_0, y_0.z_0)$ is the point with coordinates taken as the respective averages of the 60 x, y, and z coordinates, and that represents the geometric center (as well as the center of mass) of the C$_{60}$ fullerene.

$$x_0 = \frac{1}{60} \sum_{i=1}^{60} C_i(x), \quad y_0 = \frac{1}{60} \sum_{i=1}^{60} C_i(y), \quad z_0 = \frac{1}{60} \sum_{i=1}^{60} C_i(z)$$

The distance (radius) r_i from O to vertex C_i is

$$r_i = \sqrt{(C_i(x) - x_0)^2 + (C_i(y) - y_0)^2 + (C_i(z) - z_0)^2}$$

The 60 radii can be calculated in this way.

Furthermore, the distance $l_{i,j}$ between carbons C_i and C_j is

$$l_{i,j} = \sqrt{(C_i(x) - C_j(x))^2 + (C_i(y) - C_j(y))^2 + (C_i(z) - C_j(z))^2},$$

and the distances between all 60 carbons can also be calculated.

Next, using the general equation of a plane $(ax + by + cz + d = 0)$, we can check whether all five carbons of five-membered rings and all six carbons of six-membered rings lie in the same plane. Actual calculations in a spreadsheet program showed that the five-membered and six-membered rings lied not in the same planes but in a twisted configuration. Conceivably, this could be due to an error in the radius r_i from the center O to each carbon C_i.

What is the source of the twisting of the five-membered and six-membered rings and the errors in r_i and $l_{i,j}$? Is it due to measurement error or computation error? Or is it that there is no error and the scattered coordinates are the real ones and the stability of the C_{60} molecule is maintained by the 60 carbons with scattered coordinates?

Because in the truncated icosahedron all edges are of the same length and the distances from the center to the vertices are equal, all vertices lie on the surface of the same sphere. Taking the edge length as a, the radius of the circumscribed circle is

$$r = \frac{a}{4}\sqrt{58 + 18\sqrt{5}} \simeq 2.4780a$$

Strictly speaking, the C_{60} fullerene is different in shape from a truncated icosahedron (soccer ball).

This made me want to take a step further from just looking at the molecular structure in Jmol and to make an actual model of C_{60} using a molecular modeling kit. Most commercial kits have only carbon atoms and atomic bonds, and do not distinguish between single and double bonds. Even though the idea of electron delocalization is in the mainstream of modern chemistry, I thought that the idea of single and double bonds is certainly still alive, and I found the MOL-TALOU molecular modeling kit. It is sold by the Japanese company Talou Co., Ltd., whose website is http://www.talous-world.com/. This kit distinguishes between single and double bonds. This was my first ever attempt at putting together a molecular model.

4. Single and Double Bonds

The first X-ray analysis of C_{60} was done by Hawkins et al. in 1991. Each C_{60} molecule in a C_{60} crystal rotates at high speed, which makes it extremely difficult to perform an X-ray structural analysis. Hawkins et al. synthesized the C_{60} adduct $C_{60}(O_sO_4)$ (4-*tert*-buttylpyridine)$_2$ from C_{60} and O_sO_4, which stopped the rotation inside the crystal and allowed for X-ray structural analysis to be conducted on a disorder-free crystal. In this way, the positions of all carbons in the C_{60} molecule were determined. Also, they found that there are two different types of bonds with different lengths between carbons in the C_{60} molecule. The mean length of bonds connecting carbons in two different six-membered rings was 0.1388(9) nm, and that for carbons in six-membered and five-membered rings was 0.1432(5) nm [7][9].

Also in 1991, David et al. reported that the length of bonds connecting carbons in two different six-membered rings is 0.1391(18) nm, and that for carbons in five-membered and six-membered rings is 0.1455(12) nm [8]. Both studies found that the average distance between atoms in five-membered rings is about 0.005 nm longer than that between atoms in six-membered rings. This indicates that the bonds between atoms in five-membered rings are single while the bonds between atoms in six-membered rings are double. Double bonds are characterized by higher electron density and shorter bond lengths than single bonds.

The article on buckminsterfullerene on Wikipedia says that the C_{60} model differs slightly from one country to another, and the following three types are recognized (Fig. 12).

(a) A distinction is made between single and double bonds, and six-membered rings have alternating single and double bonds, like a benzene ring.

(b) A distinction is made between single and double bonds, but the double bonds are distributed among five-membered and six-membered rings without any particular rule.

(c) A distinction is not made between single and double bonds, and only the positions of the atoms are indicated.

Of these three models, (a) is used in England, Poland, and China, (b) in Spain, Japan, Iran, Indonesia, The Netherlands, and Sweden, and (c) in France, Denmark, Korea, and Italy.

Each of the representations in Fig. 12 has its advantages and disadvantages. A model showing the electron density is given in Fig. 13. This image is also from Wikipedia and shows C_{60} with ground state electron density isosurface calculated by density functional theory. This representation does not use single
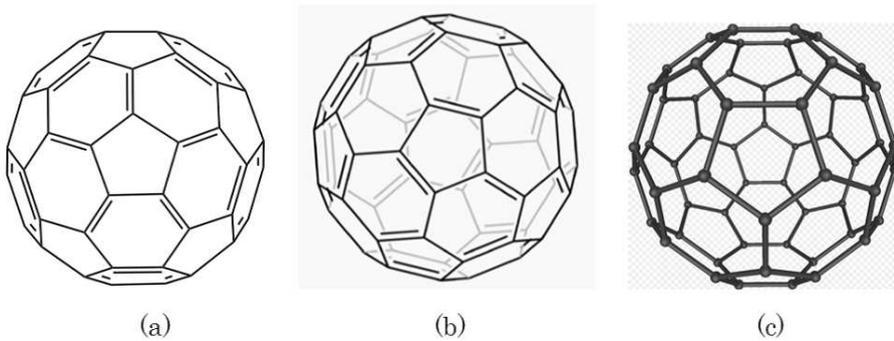
Figure 12: 12 Three representations of a C_{60} fullerene

and double bonds, but instead adds the outermost shell electrons to the model in Fig. 12 (c) in the form of an electron cloud. This is explained by the concepts of quantum chemistry.
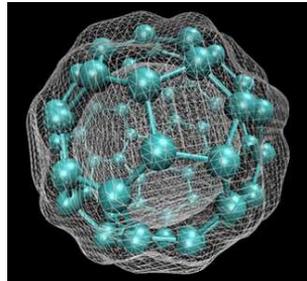

Figure 13: Electron density isosurface in C_{60} (courtesy of Wikipedia).

A carbon atom contains four valence electrons. In other words, carbon atoms can form four bonds. All carbon atoms in a C_{60} fullerene are connected to three other atoms, and because there are four bonds per three atoms, one of the bonds must be double. This is illustrated in Fig. 14. The circle represents the carbon atom, single lines represent single bonds, and the double line represents a double bond. It is considered that the carbon atom contributes one electron to single bonds and two electrons to double bonds.

In the model of the C_{60} fullerene in Fig. 12 (a) all five-membered rings consist of single bonds and all six-membered rings consist of alternating single and double bonds, but if we focus on electron delocalization, restricting the representation to such a combination of bonds is unreasonable. This is obvi-
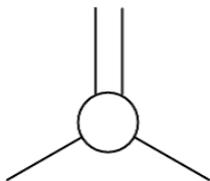
Figure 14: Two single bonds and one double bond

ous from the fact that the benzene ring can be represented in various ways. Therefore, various patterns for the five-membered and six-membered rings can be given (Figs. 15 and 16).

First, five-membered rings can have only single bonds (5a), only one double bond (5b), or two double bonds (5c). There are no other possibilities (Fig. 15).
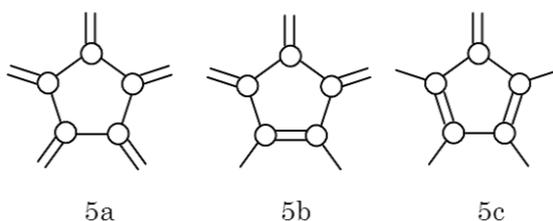

5a   5b   5c

Figure 15: The three possible combinations of bond arrangement in five-membered rings

Next, six-membered rings can have three single and three double bonds (6a), two double bonds (6b and 6c), one double bond (6d), or no double bonds at all (6e). For both five-membered and six-membered rings, the number of atomic bonds facing outward changes in accordance with the diagram in Fig. 14.

Figure 17 shows the category symbols for five-membered and six-membered rings (Figs. 15 and 16) for the structures in Fig. 12 (a) and (b). The structure in (a) contains only five-membered rings of type 5a and six-membered rings of type 6a. In contrast, the structure in (b) contains five-membered rings of type 5c and six-membered rings of types 6a, 6b, 6c, and 6d.

The regular structure in (a) and the irregular structure in (b) appear unrelated at first glance, but it is possible to show that the two types are equivalent under some operations, and it is possible to transform one type into the other
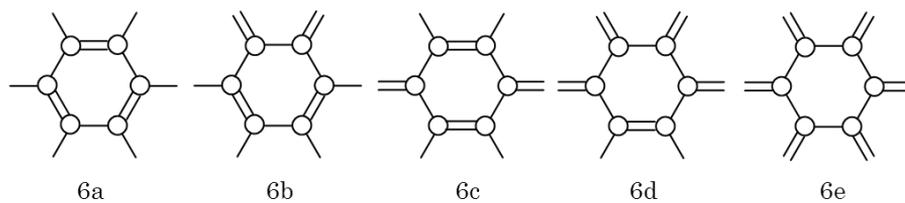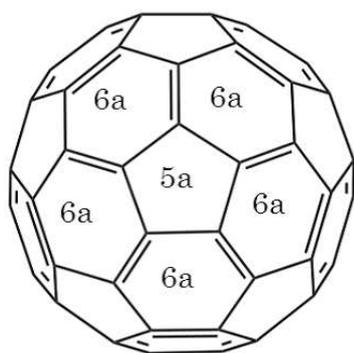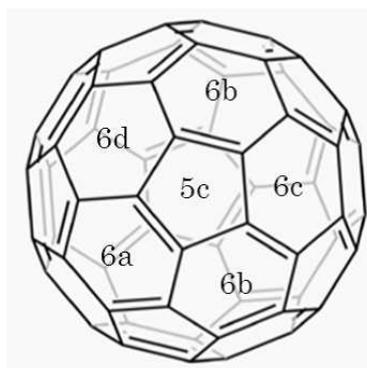
Figure 16: The five possible combinations of bond arrangement in six-membered rings

(a) Only 5a and 6a

(b) Various

Figure 17: Representations of different pattern types

(Fig. 18). For example, we can bring a six-membered ring of type 6a to the center and surround it alternatingly with five-membered rings of type 5a and six-membered rings of type 6a (Fig. 18 (a)). Because all the outward-facing bonds of the central 6-membered ring are single, rotating the ring does not affect the surrounding five-membered and six-membered rings. Therefore, rotating the central six-membered ring of type 6a by 60° yields the structure in Fig. 18 (b), where the central six-membered ring is still of type 6a but the types of the surrounding five-membered and six-membered rings change from 5a to 5b and from 6a to 6b, respectively.

By slightly changing the orientation of the balls in Fig. 18 (b), which was obtained by rotation, we can obtain the distribution in Fig. 18 (c). In other words, there are five-membered rings of types 5a and 5b as well as six-membered rings of types 6a and 6b around the central six-membered ring of type 6a. As before, all outward-facing bonds of the central ring are single, allowing it to be rotated. So, rotating the central ring by 60° gives the structure in 18 (d), where the ring of type 5b is transformed into a ring of type 5c and that of type 6b is transformed into one of type 6d.

Furthermore, rotating the central six-membered ring of type 6a in the structure in Fig. 18 (e) by 60° gives us the structure in Fig. 18 (f), where the ring of type 6d is transformed into one of type 6e.

In this way, the regular C$_{60}$ model containing only five-membered rings of type 5a and six-membered rings of type 6a can be used to generate patterns with five-membered rings of types 5b and 5c and six-membered rings of types 6b, 6d, and 6e by rotating the central six-membered ring of type 6a. This operation is similar to the operations applied to a Rubik's cube. Starting from a state where all the faces of the cube are solved (19 (a)) and rotating each face around a certain axis (Fig. 19 (b)), it is possible to get to a state where all the colors are distributed randomly (Fig. 19 (c)). A transformation from an ordered to a disordered state and vice versa can be performed through rotation.

However, we can't say that all possible combinations of single and double bonds can be obtained by rotating a six-membered ring of type 6a. For example, this operation cannot give a pattern where the double bonds are distributed at 180°, as in a six-membered ring of type 6c.

We cannot say which of the two C$_{60}$ models (a) and (b) is correct. If we assume that C$_{60}$ is generated by stacking corannulene molecules (Fig. 20), type (a) becomes plausible, and the high symmetry of this model provides an explanation for the stability of the molecule. However, type (b) is more natural if we think of C$_{60}$ fullerene as being formed from 60 scattered carbon atoms that evaporate from a graphite rod during an arc discharge. The structure in
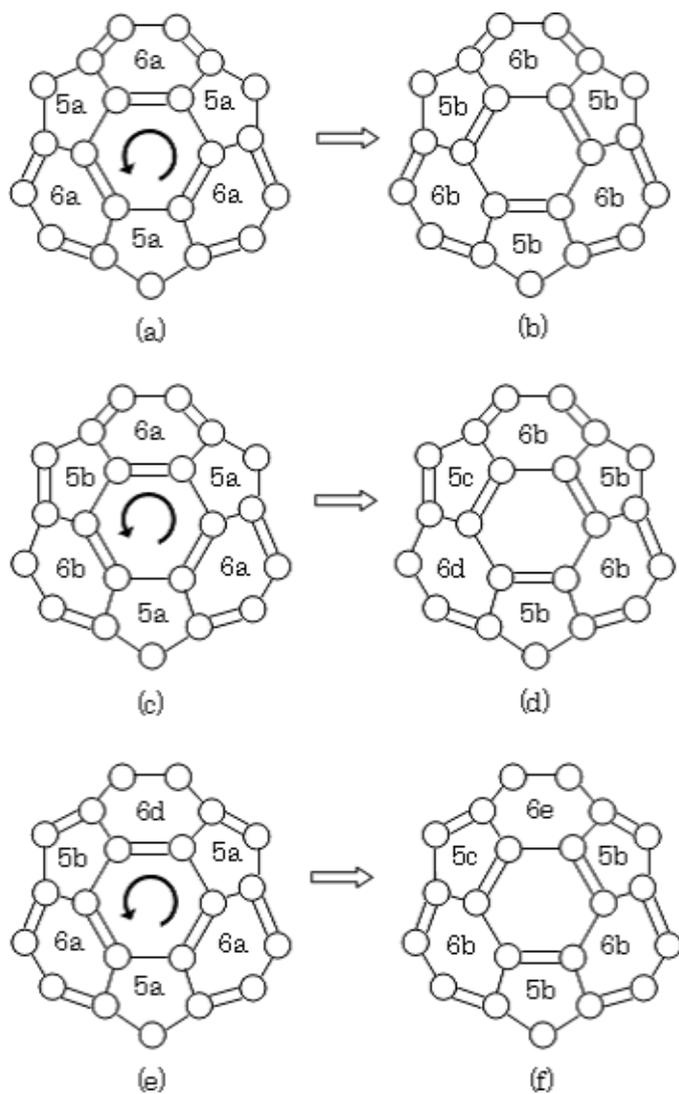
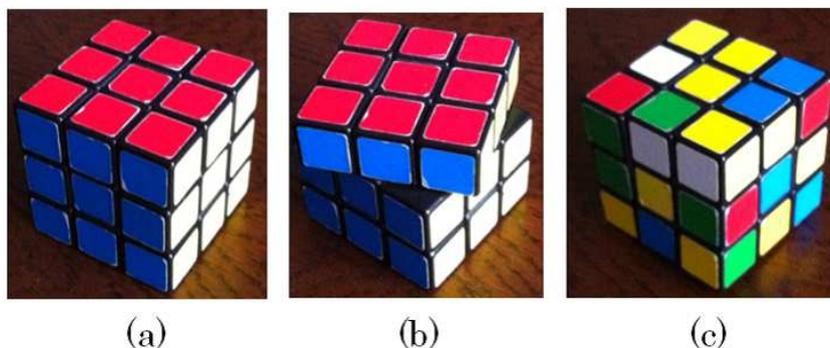Figure 18: Generating new patterns by rotating a six-membered ring of type 6a

Figure 19: Moving the faces of a Rubik's cube

Fig. 12 (a) is assumed in the articles by Hawkins et al. [7] and David et al. [8] in 1991, and that in 12 (b) has not been explained. The measurements of the length of carbon-carbon bonds are from 1991, and it is rather interesting to see how these experimental values are evaluated at present, more than 20 years later.

Structure type (c), which disregards the distinction between single and double bonds, shows the positions of the carbon atoms but does not provide any explanation of the fact that the valence of the carbon atom is 4 (i.e., it forms four bonds). Since I am not an expert, let's not go any further into a discussion about which of the three structures (a), (b), or (c) is correct.
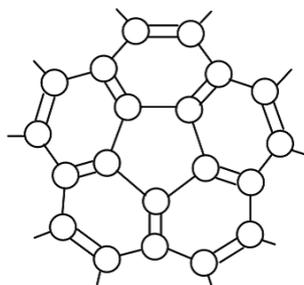

Figure 20: Corannulene ($C_{20}H_{10}$)

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