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Program 'FULLER' for producing isomeric fullerene structures from their projections

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Using formalized projection of fullerene structure on 2D-triangular lattice, we have developed a program package which outputs topological Cartesian coordinates of the fullerene, useful for the input of further theoretical calculations. The package is capable of producing an infinite number of structures of homologous fullerene.

1. INTRODUCTION

Fullerenes are closed polyhedra consisting of sp^2-hybridized carbon atoms. They have complicated network of 5-membered and 6-membered rings of a large number of carbon atoms. We can hardly draw structures or generate coordinates by hand, hence computer drawing is the natural choice. However, available 2D- or 3D-modelling software packages are not flexible enough to treat the ever expanding new members of fullerene family.

We have already reported that the structure of any fullerene can be described as a projection onto 2-dimensional lattice[1] and that the projection drawn by certain fixed procedure can be conveniently used for generating infinite number of homologous fullerene structures.

In this paper, we mention a package of programs which incorporate the projection algorithm and include automatic generation routine of atomic Cartesian coordinates. These programs have been placed for public use[2].

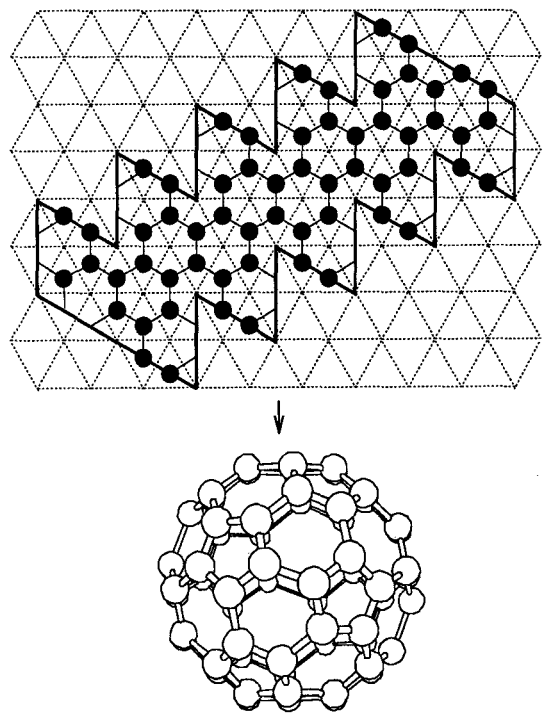

Figure 1. Projection and 3D model of I_h-C_{60}.

2. PROJECTION OF THE FULLERENES

Fullerenes of I-symmetry such as buckminsterfullerene (C_{60}) are geometrically equivalent to Goldberg polyhedra[3, 4]. Because the Goldberg polyhedra derive from icosahedron, a projection of icosahedron (bold line, Figure 1) can be used for projecting I-symmetric fullerenes. Actually, a paper model of I_h-C_{60} can be readily constructed by cutting out and folding the projection of Figure 1, and placing carbon atoms at each center of small triangles. Twelve corners in the projection become the centers of twelve pentagons. For this reason, the corners are called 'pentagonal defects' [5]. Cross points on the triangular lattice become the center of hexagonal carbon ring in fullerenes.

As mentioned before[1], it is advantageous, for subsequent generation of fullerene structures with low symmetry and their atomic coordinates, to regard a projection as composed of a central 'band'

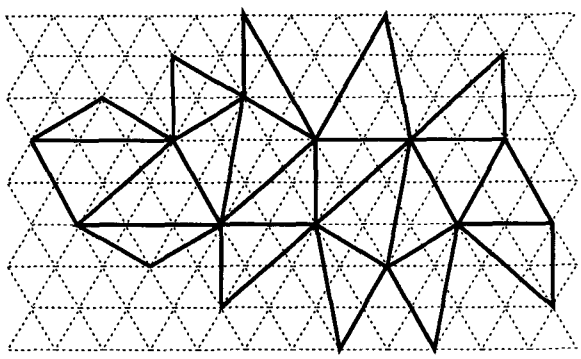

Figure 2. Projection of C_1-C_{84}.

containing ten triangles and a pair of 'cap' structures, each cap containing six corners. In general, there is no need for all of the triangles in a projection to be regular triangles, if the projection can be folded into a solid. Figure 2 gives an example of projection consisting mostly of non-regular triangles, which gives upon cutting and folding a C_{84} fullerene having no any symmetry element. Note that the band area is no longer a parallelogram.

3. GENERATION OF ISOMERS

One particular projection corresponds to a fullerene structure. We utilize this one-to-one correspondence to produce isomeric and homologous structures of fullerenes by first generating as many projections as possible and then deriving different fullerene structures from them. For this purpose, we wrote the following three programs for

(1) Generating various cap structures,

(2) Combining a pair of cap structures above and below a band structure such that the resulting projection can be folded into a solid consisting of twelve pentagons and various number of hexagons,

(3) Finally producing atomic Cartesian coordinates of the corresponding fullerene from the projection (Figure 3).

3.1. Caps

A cap is a row of five triangles connected at the corner like those shown in Figures 1, 2 and

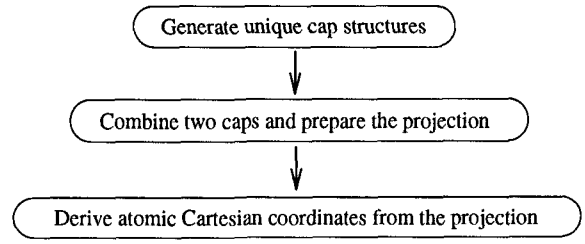

Figure 3. Flow chart of isomer-generating.

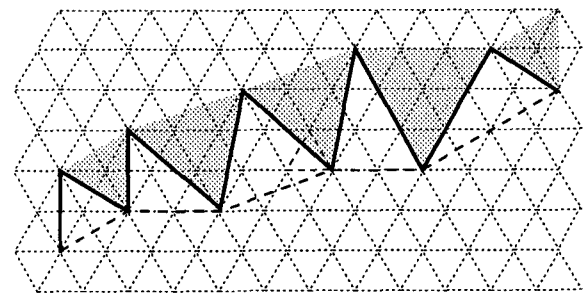

Figure 4. An example of cap structure.

4. As mentioned above, there is no restriction on the shape and size of triangle. In order that a cap folds itself to form a part of solid containing six 'pentagonal defects', two facing edges of a pair of connected triangles must be of the same length and the solid angle around a lower corner must be 300°. In other words, those parts of lattice (Figure 4, shadowed) which will be cut off and thrown away when the projection is to be folded, must be regular triangles. Taking advantage of the latter fact, we reduce the problem of generating all possible unique cap structures to that of exhaustively finding unique combinations of five regular triangles of any size. Such regular triangles are the components of Goldberg polyhedra[3, 4].

Figure 5 illustrates the process of generating cap structures. First, componential regular triangles of different sizes are prepared and named in the order of increasing area (A, B, C $\cdots$ Figure 5(a)). A combination of five regular triangles from this file, allowing any repeated sampling, and disallowing overlap of edges between the adjacent triangles, produces a cap (Figure 5,(b)). When the isolated pentagon rule (IPR) is to be

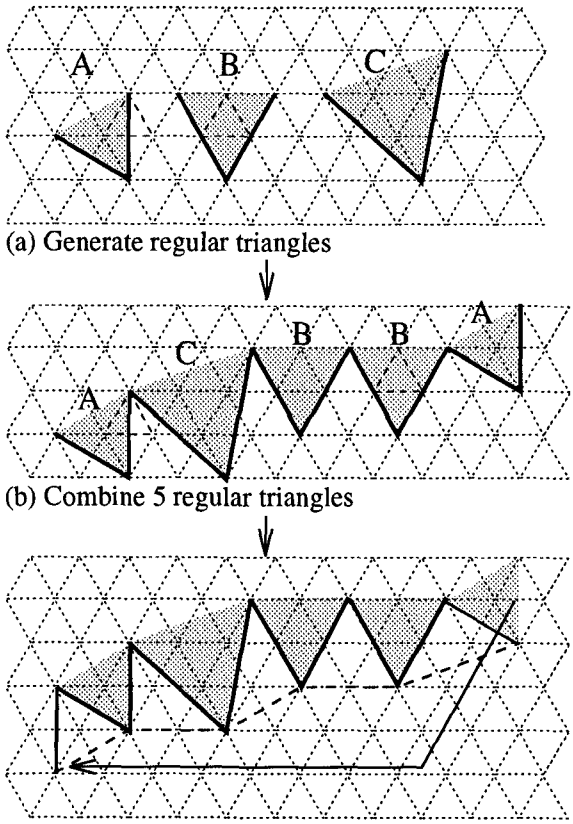

Figure 5. Process of generating a cap structure.

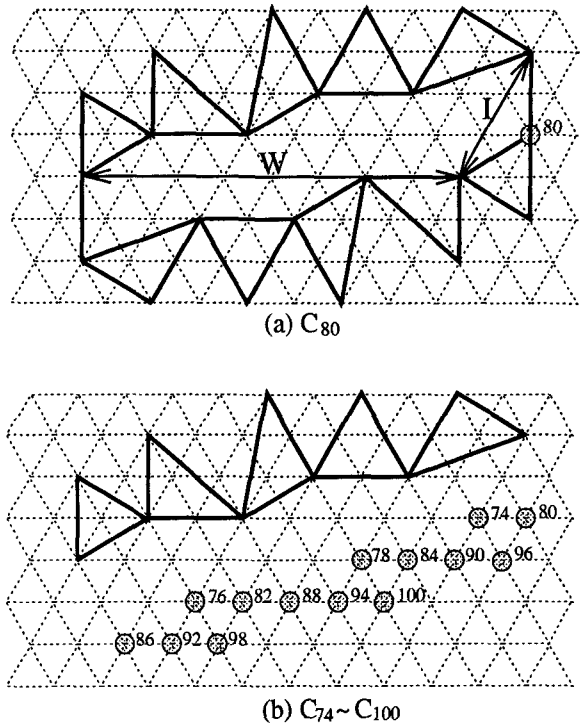

Figure 6. Fullerene isomers that can be derived from one pair of cap structure.

preserved, the distance of neighbouring corners should be longer than 1. The present version of program takes care of IPR.

Figure 5(b) presents a combination of ACBBA triangles. The number of combinations increases sharply with the number of componential triangles. Our program takes care of creating all possible combinations, transferring the edge at the right end to the far left end to complete the cap structure, and removing duplicate structures (Figure 5(c)).

3.2. Projection

A pair of cap structure can be used for a projection, if they have the same inclination I and width W (Figure 6a). Clearly any cap and its 180°-rotated copy provide a projectable pair (figure 6a). Both vertical sides of a band must be parallel and of equal height for the projection to fold into a solid. Hence, if the right-end corner of the lower cap (marked with ◎) is placed as shown in Figure 6a, the position of the left-end corner is automatically decided as shown to give a projection for an isomer of C_{80} fullerene. Figure 6b shows *fourteen* possible positions of the right-end corner to produce fullerenes smaller than C_{100}. Actually any eligible pair of cap structure can produce literally infinite number of projections for fullerenes by changing the position of band.

3.3. Cartesian coordinates

Using the projection thus obtained, we can generate atomic Cartesian coordinates according to the method of Manolopoulos and Fowler[6]. One of our programs that performs this function is named FULLER.

Input for FULLER requires only the contour of projection, namely a set of coordinates of 22 corners (Figure 7a). The contour is then divided into twenty triangles(b). Thereupon carbon atoms are placed at the center of every small triangle and

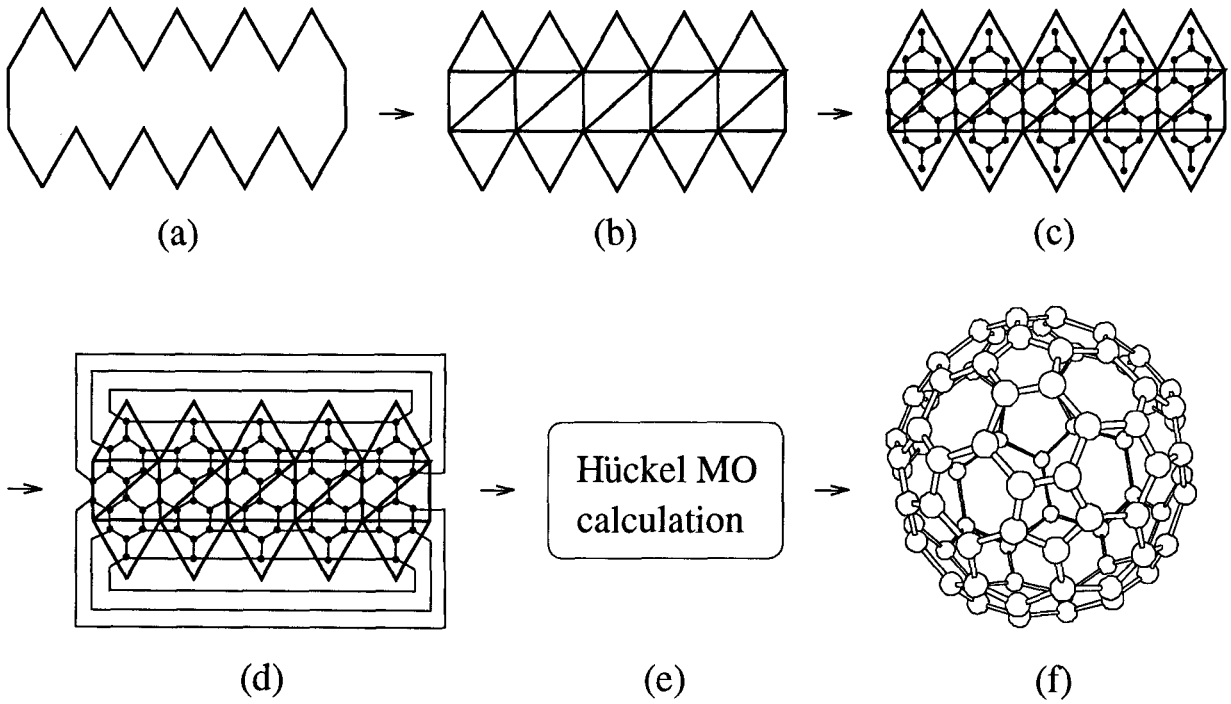

Figure 7. The algorithm of FULLER.

the connectivity among atoms are deduced based on the calculated interatomic distances (c). Connection between the both ends of cap is determined by the rotation and translation of triangles concerned (d). A large part of the source code in FULLER pertains to the step d.

Once the atomic connectivity is known, we can readily write down secular determinant for Hückel molecular orbitals of the fullerene. In the program FULLER, HMO calculations are performed automatically (e). There are three occupied HMO's which have only one node and orthogonal against each other. Their eigenvalues are assigned to X, Y, and Z coordinates, respectively, of each atom, and are then appropriately scaled to give a set of topological Cartesian coordinates suitable for an input of molecular mechanics or semi-empirical molecular orbital calculations (f). The number of nodes in a HMO's can be determined by using the eigenvector and connectivity. Namely, all the bond across which the sign of atomic coefficient (zero is regarded as positive) changes are cut and in the end the number of molecular fragments are counted to obtain the number of nodes. Eigenvalues are used for judging duplication.

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