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A Note on a Variant of the Leapfrog Transformation of Chemical Graphs*

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A variant of the leapfrog transformation is discussed. It is pointed out that the presented variant of the leapfrog transformation is a powerful graph-theoretical technique for generating many classes of (chemical) graphs. This technique is applied to polyhexes, square animals and other planar polycyclic graphs with cycles of various sizes.

The leapfrogging technique was introduced for systematic generation of fullerenes.[1-7] A given fullerene C_n of n carbon atoms can be always used to generate a larger fullerene C_{3n} with $3n$ carbon atoms by the leapfrog transformation. The leapfrogging technique is actually a very powerful graph-theoretical technique which can be used for generating many different classes of graphs.

In this report, we wish to discuss a variant of the leapfrogging technique and describe its application to several classes of planar polycyclic graphs. This variant of the leapfrogging technique consists of two steps: the first step involves the omnicapping process[8] and the second step the construction of the inner dual.[9] The variant differs from the original proposal in using the inner dual instead of the dual.

Let us call the initial polycyclic (polygonal) graph the *parent graph*. The omnicapping process (which is also called the stellar subdivision) consists of putting a

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vertex (planting a seed) in the center of each face (polygon) of the planar embedding of the polycyclic graph and then connecting it with the vertices of a polygon. This process produces a deltagonal polycyclic graph for the parent graph. We call the deltagonal polycyclic graph the *delta graph*. All faces in the delta graph are trigonal. The first step of the leapfrog transformation ends with the creation of the delta graph. This process is illustrated in Figure 1 for the case of the heptagon.

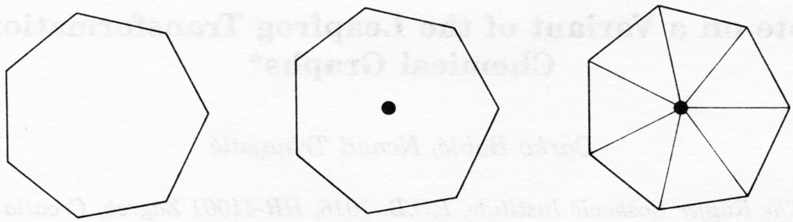

Figure 1. The omnicapping process.

The inner dual can be constructed in the following way:[9] Place one vertex in the center of each face and, if two faces have an edge e in common, join the corresponding vertices with an edge e^* crossing only e. Construction of the inner dual of the deltatetrabenzoanthracene graph (*i.e.*, the dualization of the delta graph) is shown in Figure 2.

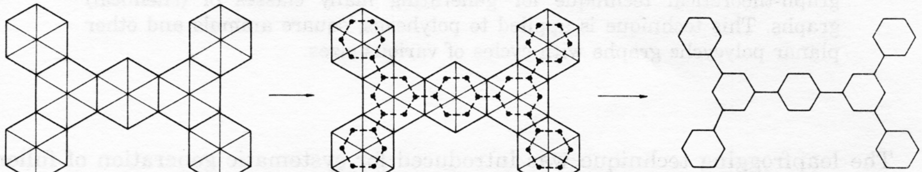

Figure 2. Construction of the inner dual of deltatetrabenzoanthracene graph, *i.e.*, dualization of the delta graph.

The inner dual operation gives a novel polycyclic graph from the delta graph, called the *leapfrog graph*. An important point to emphasize is that the symmetry characteristics of the parent graph and its leapfrog graph match, unless there are bridges in either of these two graphs. The leapfrog transformation may be schematized as:

$$\textbf{parent graph} \xrightarrow{\text{omnicapping process}} \textbf{delta graph} \xrightarrow{\text{construction of the inner dual}} \textbf{leapfrog graph}$$

Below we describe the use of the above procedure on several classes of chemical graphs.

(i) The leapfrogging of polyhexes

Dias[10] first used the leapfrog transformation outside the fullerene domain. Dias has used it for generating polyhexes.[10,11] Polyhexes are planar graphs that may be obtained by any combination of regular hexagons, such that two of its hexagons have exactly one common edge or are disjoint.[12] Dias has shown that any simply connected polyhex (*i.e.*, polyhex without holes) with n vertices can be transformed by the leapfrog method into a successor polyhex or nonpolyhex graph (such as biphenyl) with $[3(n - V_2) + 6]$ vertices (V_2 = the number of vertices with the degree equal to 2). If the result is a polyhex, it contains the maximum number of Clar sextets[13] and the same point symmetry group as the parent graph.

In Figure 3 we give the leapfrog transformation of a triangulene graph into a tribenzo[a,g,m]coronene graph. The corresponding conjugated hydrocarbons are open-shell and closed-shell structures, respectively.

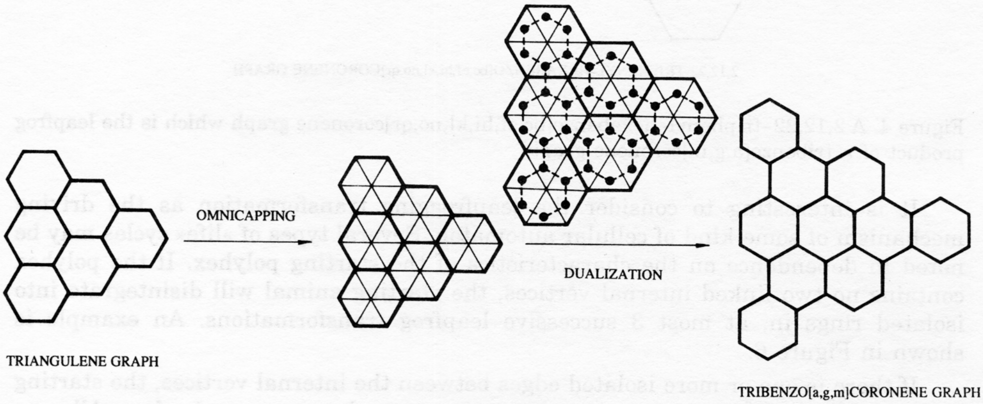

Figure 3. The leapfrogging of a triangulene graph into a tribenzol[a.g.m]coronene graph.

The tribenzo[a,g,m]coronene graph can produce, by an additional leapfrog transformation, a 2,12,22–triphenyl–hexabenzo[bc,ef,hi,kl,no,qr]–coronene graph (see Figure 4), which is again a closed-shell polyhex but this one cannot further procreate into another polyhex.

We note that the leapfrog transformation of benzene leads back to benzene (rotated by 30° from its original orientation). This is the null leapfrog.

In Figure 5, we give the leapfrog transformation of a simple coronoid graph (*i.e.*, multiply-connected polyhex) with 8 hexagons. The end product of this leapfrogging is a cyclic graph, also with eight hexagons. However, this graph is no longer a polyhex. We note that any coronoid with n vertices can be transformed by leapfrogging into cyclopolyphenyl with $3(n{-}V_2)$ vertices.

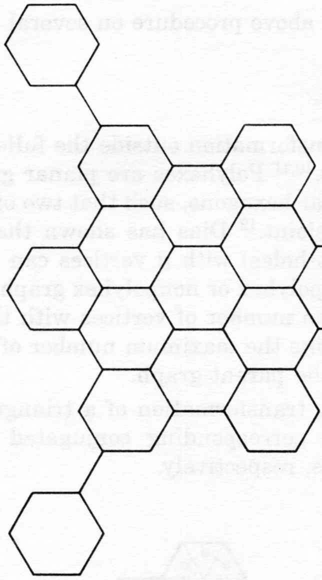

Figure 4. A 2,12,22–triphenyl–hexabenzo[bc,ef,hi,kl,no,qr]coronene graph which is the leapfrog product of a tribenzo[a,g,m]coronene graph.

It is interesting to consider the leapfrogging transformation as the driving mechanism of some kind of cellular automaton. Several types of »life« cycles may be noted in dependence on the characteristics of the starting polyhex. If the polyhex contains no two linked internal vertices, the starting animal will disintegrate into isolated rings in, at most 3 successive leapfrog transformations. An example is shown in Figure 6.

If there is one or more isolated edges between the internal vertices, the starting polyhex will break away into as many components as there were such edges. All components are equal and repeating the leapfrog operation makes them oscillate with spitting out free hexagons, as shown in Figure 7.

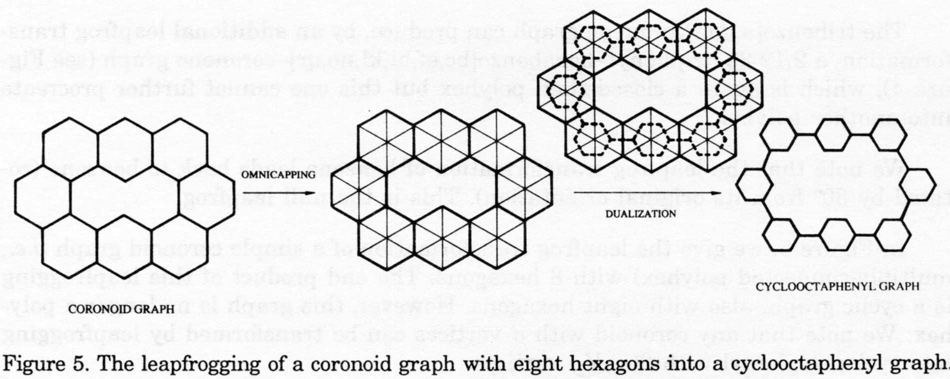

Figure 5. The leapfrogging of a coronoid graph with eight hexagons into a cyclooctaphenyl graph.

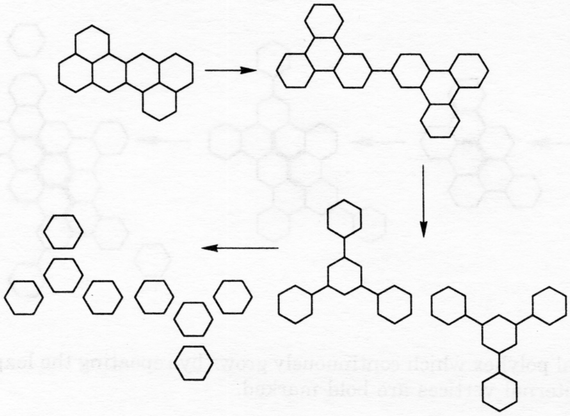

Figure 6. A polyhex which disintegrates into free hexagons by repetitive leapfrogging.

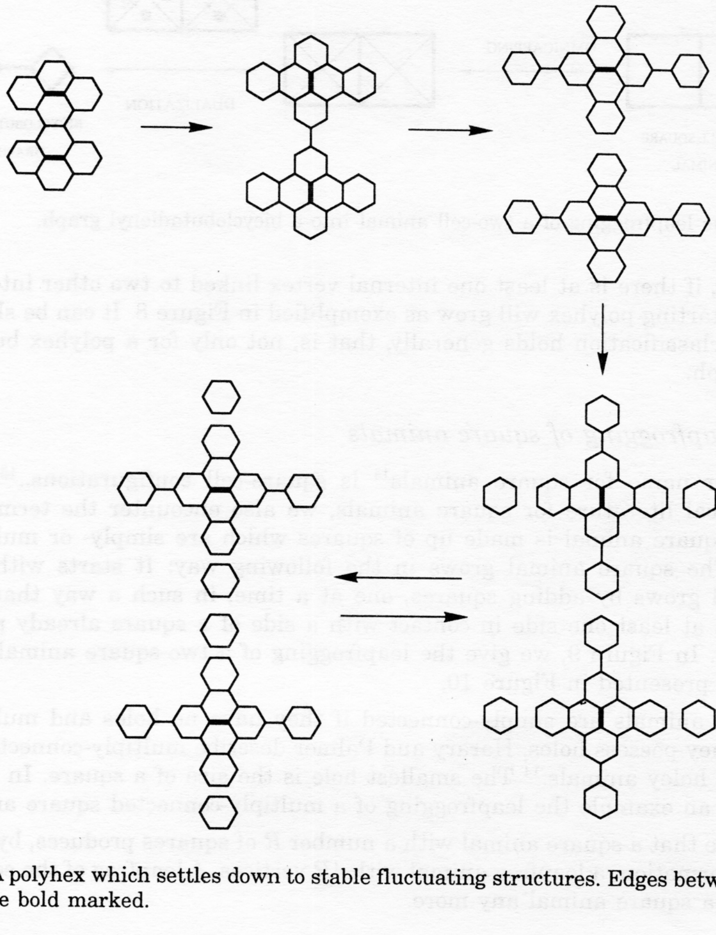

Figure 7. A polyhex which settles down to stable fluctuating structures. Edges between internal vertices are bold marked.

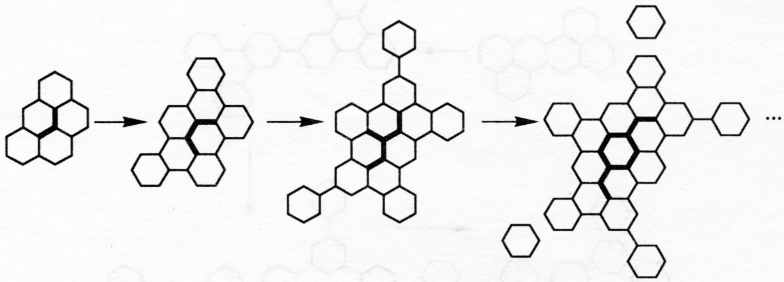

Figure 8. A minimal polyhex which continuously grows by repeating the leapfrog operation. Edges between the internal vertices are bold marked.

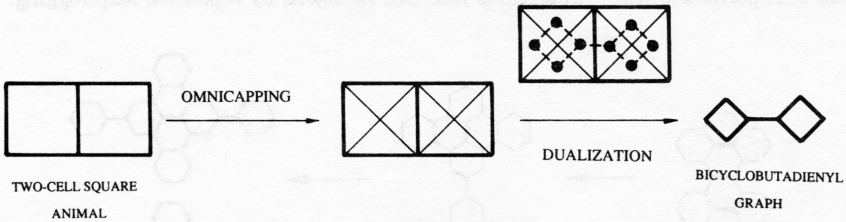

Figure 9. The leapfrogging of a two-cell animal into a bicyclobutadienyl graph.

Finally, if there is at least one internal vertex linked to two other internal vertices, the starting polyhex will grow as exemplified in Figure 8. It can be shown that the above classification holds generally, that is, not only for a polyhex but for any planar graph.

(ii) The leapfrogging of square animals

Another name for square animals[14] is square-cell configurations..[15,16] In the mathematical literature for square animals, we also encounter the term polyominoes.[17] A square animal is made up of squares which are simply- or multiply-connected.[18] The square animal grows in the following way: It starts with a single square and grows by adding squares, one at a time, in such a way that the new square has at least one side in contact with a side of a square already present in the animal. In Figure 9, we give the leapfrogging of a two-square animal. Another example is presented in Figure 10.

Square animals are simply-connected if they have no holes and multiply-connected if they possess holes. Harary and Palmer describe multiply-connected square animals as holey animals.[14] The smallest hole is the size of a square. In Figure 11 we give as an example the leapfrogging of a multiply-connected square animal.

We note that a square animal with a number R of squares produces, by the leapfrog transformation, a leapfrog animal with $4R$ vertices. A leapfrog of the square animal is not a square animal any more.

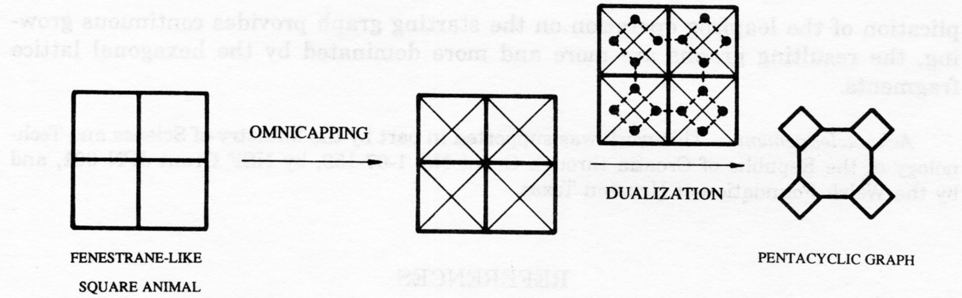

Figure 10. The leapfrogging of a fenestrane-like square animal into a pentacyclic graph consisting of four 4-membered cycles and one 8-membered cycle.

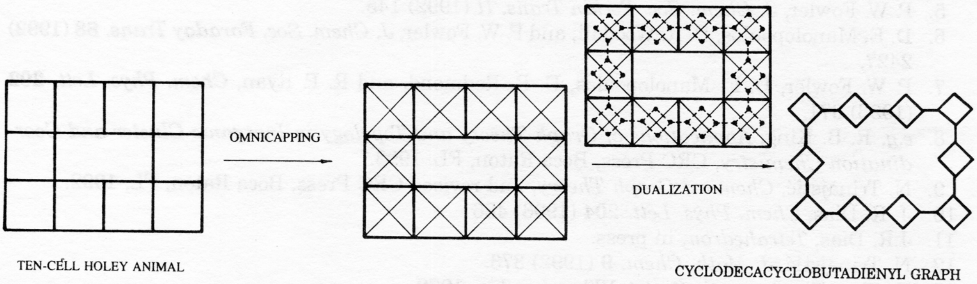

Figure 11. The leapfrogging of a holey animal with 10 squares into a cyclodecacyclobutadienyl graph.

(iii) The leapfrog of polycyclic graphs with rings of various sizes

The leapfrog transformation can be applied to any planar polycyclic graph without any difficulty. In Figure 12 we depict the leapfrogging of an azulene graph. The leapfrog product of the azulene graph is a sesquifulvalene graph.

Note that all vertices in the leapfrog graph are either di- or trivalent, and that the only new rings produced by the leapfrog operation are hexagons. Repetitive ap-

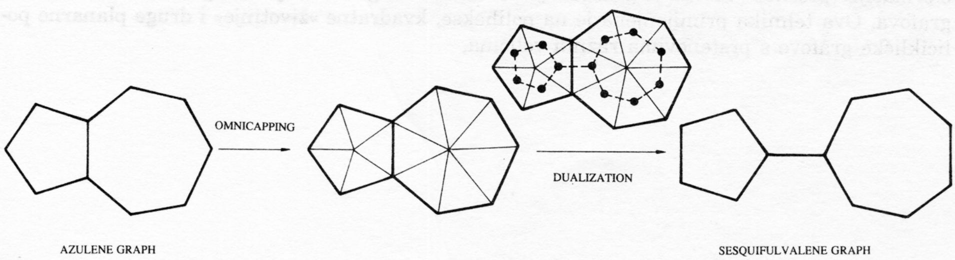

Figure 12. The leapfrogging of an azulene graph into a sesquifulvalene graph.

plication of the leapfrog operation on the starting graph provides continuous growing, the resulting graphs are more and more dominated by the hexagonal lattice fragments.

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SAŽETAK

Bilješka o varijanti »preskok« transformacije kemijskih grafova

Darko Babić, Nened Trinajstić i Douglas J. Klein

U radu je razmatrana jedna varijanta transformacije »preskok«. Prikazana varijanta transformacije »preskok« moćna je graf-teorijska tehnika za generiranje mnogih klasa (kemijskih) grafova. Ova tehnika primijenjena je na polihekse, kvadratne »životinje« i druge planarne policikličke grafove s prstenovima raznih veličina.