A Catalogue of Growth Transformations of Fullerene Polyhedra

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Carbon insertion or extrusion mechanisms transforming one fullerene to another are presented as patch replacements on the fullerene surface. A systematic catalogue is constructed for the topologically distinct local insertion/extrusion transformations of fullerenes, classified by patch boundary and pentagon content. All pairs of patches with the same boundary but different numbers of atoms, i.e., growth patches, containing up to five pentagons, with an upper limit for the boundary length that depends on the number of pentagons, are listed. New transformations and infinite series of transformations are identified.

INTRODUCTION

The definition of a fullerene as a polyhedral carbon cage C_n with all atoms directly bonded to three others, and with all faces either pentagonal or hexagonal, is consistent with a multiplicity of isomers and an infinite range of nuclearities. Fullerene polyhedra are mathematically possible for $n = 20 + 2h$ ($h \neq 1$) vertices,[1] and the 12 pentagons and $h = n/2 - 10$ hexagons of the cage can be arranged in multiple isomeric forms for all $n \geq 28$.[2] Chemical attention focuses on the isolated-pentagon fullerenes, which are possible for $n = 60$ and $n \geq 70 + 2h$ ($h \geq 0$), with multiple isolated-pentagon isomers for $h \geq 3$, and which typically have greater thermodynamic stability than isomers of comparable size with adjacent pentagonal faces.

Transformations between isomeric fullerenes at fixed n, or between fullerene polyhedra that differ in number of vertices, are of mathematical interest as defining interconversions of polyhedra and as a means of grouping fullerenes into related classes, but they also offer models of chemical and physical processes of isomerization and growth.

Isomerization via the Stone−Wales transformation[3] or other processes has been invoked as a possible explanation of the observation that the fullerene cages obtained in experiment by chromatographic separation from the products of the Krätschmer-Huffman synthesis correlate well with predictions for the thermodynamically preferred isomers at the observed values of n. Thermal annealing of high-energy forms to yield more stable isomers, albeit by processes that pass over high activation barriers, offers a rationalization. Transformations in which carbon atoms are added to or subtracted from fullerene cages in multiples of two[4] are of interest for construction of fullerene-road[5] models of fullerene formation, in description of carbon ingestion steps in nanotube growth, and in accounting for the mass spectra produced in laser-induced shrink-wrapping of empty fullerenes and fullerenes containing endohedral metal atoms.[6]

Previous work has established the utility of the notion of patch replacement as a common framework for representation and classification of isomerization and growth/carbon-loss transformations. A systematic catalogue of isomerization transformations based on this approach has been constructed.[7] Similar reasoning is applied here to classify the transformations that lead from an isomer of a fullerene C_n to an isomer of a fullerene C_{n+2m}. A comprehensive catalogue of combinatorially distinct growth and carbon-loss mechanisms ordered by patch boundary and pentagon content is thereby made possible.

Much of the mathematical approach is common to isomerization and growth mechanisms, and only a brief summary of background and algorithmic considerations is given here before presenting the new catalogue. As with the previous catalogue of isomerization transformations,[7] step-by-step enumeration uncovers many possibilities that have not yet received attention in the chemical literature, and it gives a firm basis for future evaluation of hypothetical mechanisms using explicit quantum chemical calculations.

The need for a systematic graph-theoretical approach to both isomerization and insertion/extrusion processes has been noted in the literature.[8,9] Just as the catalogue of isomerizations generalizes the simplest isomer interconversion, the Stone−Wales or pyracylene transformation,[3] the new catalogue generalizes the simplest growth proposal, the Endo−Kroto C_2 insertion.[4] With just one isomerization and one growth step it has been possible to construct a plausible fullerene road connecting the smallest possible hexagon-containing fullerenes with the abundant C_{60} (and C_{70}) species by a downhill (non-uphill) route;[10] combination of the two catalogues allows for the full generality of such isomerization/growth route maps.

BACKGROUND

The motivation for the representation of fullerene-to-fullerene transformations by patch replacement is that this gives a local process, which can be supposed to take place

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with breaking and forming limited numbers of bonds, and hence with physically reasonable activation energies, and in a generic fashion that may apply to any isomers containing appropriate structural motifs. In practice, as the patch size can be allowed to be arbitrarily large, the distinction between local and global transformations is a loose one. In our approach, a patch is defined as follows.[7] The surface of the starting fullerene polyhedron is partitioned into two parts by a closed boundary circuit of vertices and edges, drawn such that all changes necessary to the conversion of the initial into the final fullerene are confined to the interior of the disklike region enclosed by the boundary. Each vertex in the boundary is incident with two edges lying wholly in the boundary and one edge that points either inward to the interior or outward to the exterior region. Denoting the in and out possibilities by 1 and 0, respectively, the boundaries are labeled with binary codes, leading to a natural lexicographic ordering criterion for establishing the distinct possible boundaries and establishing their canonical codes. The patch is then constituted by the boundary circuit and all the interior vertices and edges.

A transformation of one fullerene to another can be imagined as a formal cut-and-paste operation in which the patch is cut along its boundary, lifted out of the fullerene, and replaced by another that fits the same boundary, i.e., by another patch that has the same canonical boundary code.

Isomerization transformations correspond to replacement of the original patch by either (i) a rotated or reflected copy of itself or (ii) a nonisomorphic patch with the same number of vertices and edges as the original. These cases of isomerization patches ((i)) and isomerization pairs ((ii)) have been considered previously.[7]

The third possibility is that of the formal replacement involving a new patch with a different number of vertices. This corresponds to inflation or deflation of the fullerene (necessarily by an even number of vertices), and the two patches are said to form a growth pair or an inflation pair. With isomerization processes, some care is needed to distinguish between real and null transformations.[7] Processes of type (iii) suffer from none of these difficulties, as the initial and final fullerenes are certain to have nonisomorphic graphs.

Patch replacement is a combinatorial description of the interconversion process, and in the physical fullerene molecule the transformation will be attended by potentially considerable geometric relaxation within and beyond the patch boundary and may take place in a concerted fashion or sequentially, with intervention of catalytic or chaperone species. All these subtleties are ignored in the simplified before-and-after combinatorial representation of the process. Geometric reorganization is likely to be especially significant in inflation/deflation transformations and may have consequences for physical energetics which are ignored in the purely graph theoretical approach. However, the construction of the catalogue can serve as a firm basis for further systematic quantum mechanical study of these important physical aspects.

In constructing a catalogue, several potential problems arise and must be solved by making appropriate technical definitions. If the construction of patches were allowed to range without restriction over all possible simply connected groups of pentagons and hexagons, a given transformation could appear many times in superficially different guises.
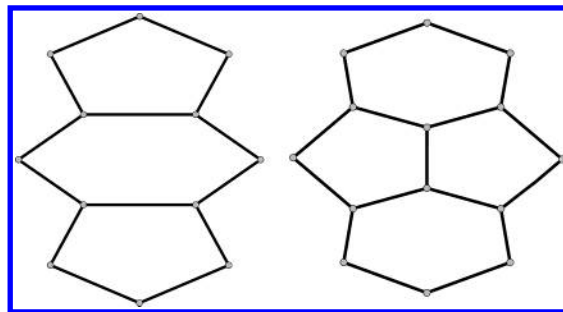

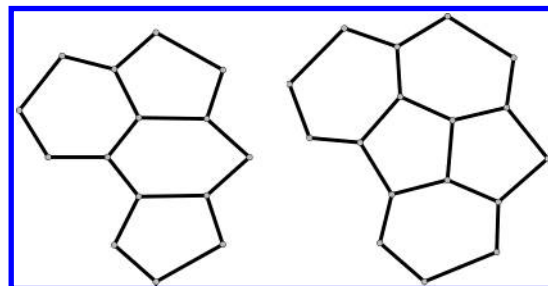**Figure 1.** The Endo−Kroto growth pair.[4]

Figure 2. The Endo−Kroto growth pair with a spectator face.

For example, the Endo−Kroto growth pair (Figure 1), the pair with an extra spectator hexagon at the same place on the boundary (Figure 2) or even its circumscription with one or more layers of hexagons all correspond to what it is intuitively clear are versions of one and the same transformation; all these versions differ only in a number of "spectator faces". To avoid this problem of redundancy, we define the notion of an *irreducible growth pair*. A growth pair is called *irreducible* if there is an isomorphism of the boundaries (that is a one-to-one mapping preserving adjacencies and vertex degrees) that does not map the boundary segment of any *removable* face onto that of another removable face of the same size. A removable face is a face in the boundary that can be removed without disconnecting the patch. It should be noted that the boundary length may either shrink or grow after such removal(s), depending on how any removed face was connected with the boundary.

Of course the irreducible growth pairs are not necessarily independent. If, say, for patches *a*, *b*, and *c* the pairs (a, b) and (a, c) are both irreducible growth pairs, the replacement (a, c) may also be obtained by first applying (a, b) and then a third, smaller operation. The patches G2.16.2.1 to G2.16.2.3 in our catalogue give an example for this with the third operation, the Endo−Kroto pair. Also note that, under this definition, unions of irreducible pairs can occur as larger irreducible pairs. A combination of Endo−Kroto growth pairs that is irreducible in our sense is given in Figure 3. This combination introduces C_4 as a pair of C_2 insertions, which could clearly be added separately (sequentially) as they take place in separate subregions of the patch, whereas the elongations of the two-pentagon Endo−Kroto patch described by Curl[11] (see also Figure 2 of ref 2, chapter 7) introduce exactly C_{2n}, rather than a sequence of n C_2 insertions.

A final and crucial restriction on the patches that are to be included in the catalogue is that they should be embeddable in a fullerene. A pair such as the one shown in Figure 4, which would be acceptable as the skeleton of a polycyclic hydrocarbon, cannot be present in a fullerene as the large bay demands at least a heptagon to fill it.
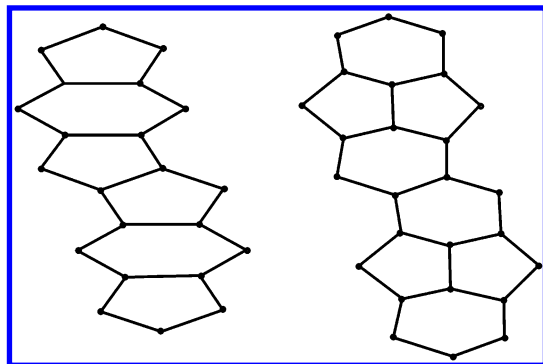
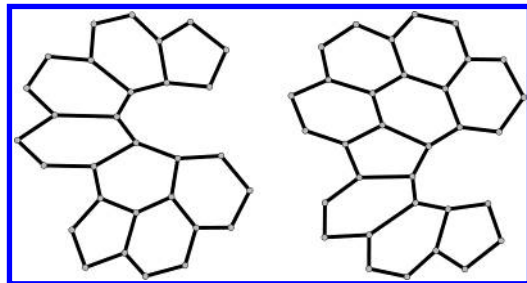**Figure 3.** An irreducible combination of two Endo−Kroto growth pairs.

Figure 4. A growth pair with patches that cannot occur in fullerenes.

Embeddability is easily decided by inspection in small cases, but to check that some hidden nonlocal restriction on embeddability was not being missed, we searched for examples of fullerenes containing any given candidate patch. All patches in the tables occur in fullerenes with at most 40 vertices.

Interpreting the patches as planar polycyclic hydrocarbons with a hydrogen attached to every boundary vertex of valency 2, it is easy to prove that the number y of hydrogen atoms for a given boundary length l and number of pentagons p is given by $y = (l + 6 − p)/2$. In Theorem 2.3 of ref 12 it was first mentioned that for a given boundary only a finite number of fillings exist.

In refs 13 and 14 it was proved that for a fixed number h of hexagons and $p \leq 6$ of pentagons a patch (in the sense used above, that is with all interior vertices of valency 3 and all boundary vertices of valency 2 or 3) with the shortest possible boundary can be obtained by gluing the faces to each other in a spiral fashion starting with the pentagons, while a patch with the longest possible boundary is obtained by gluing them in a tree-like fashion.

From this result, for every l and $p < 6$ we can determine the maximum and minimum numbers of C-atoms of a planar polycyclic hydrocarbon with boundary length l.

Our algorithm now works as follows. The boundary length l and the number p of pentagons are given as input. Then every formula C_xH_y corresponding to l and p is computed, a generator for planar polycyclic hydrocarbons (see ref 15) is started for that formula, and the output structures are examined for their symmetry group and boundary encoding. The boundary encoding is stored in order to be able to determine those encodings for which nonisomorphic fillings exist (i.e. to find which boundary encodings occur more than once).

In a second run, the same structures are generated again, but this time those that correspond to boundary encodings that occurred more than once are stored, and pairs are formed and tested for irreducibility by checking all possibilities of mapping the boundaries onto each other. Irreducible pairs are output.

Unfortunately no independent results are known to us, so we are reluctant to claim completeness of our list and do not give numbers beyond those cases presented in the catalogue as shown in Chart 1 for which the boundary structure and reducibility can be checked by hand. An independently implemented approach, preferably even using an independent algorithm (e.g. constructing all possible boundary encodings and filling them in every possible way), would give a useful check of the results presented here.

For $p = 0$ Guo, Hansen, and Zheng[16] have proved that the number of faces within a boundary is determined uniquely by the boundary, and from this it follows that no growth pairs with $p = 0$ can exist. In fact, a stronger result has been proved: the number of faces in any patch consisting of faces of any single size, with any (constant) vertex degree of the inner vertices that is an upper bound for the degree of the boundary vertices, is determined by the boundary.[17]

For $p = 1$ our computer approach did not find any growth pairs. This suggested that for $p = 1$ the number of faces inside a patch might also be determined by the boundary. A proof of this result will appear elsewhere.[18] An implication is that fullerenes with large distances between any pair of pentagons (e.g. large icosahedral fullerenes) cannot be constructed by the local replacement method applied to growth patches without using very large patches. It is not known whether isomerization patches with fewer than two pentagons can in fact occur in fullerenes. We conjecture that this is not the case. Furthermore, there is no finite basis set of fullerenes and finite repertoire of growth pairs such that *every* fullerene could be constructed using only fullerenes from the basis set and these growth pairs. There is in this sense no universal fullerene seed from which all can grow by repetitions of a finite set of such patch replacements.

THE PATCHWORK CATALOGUE

In the catalogue the patches are listed according to the number of pentagons and the boundary length. A patch with

Figure 5. Patches with three pentagons and boundary code 0001001010100010001111. The irreducible pairs are (1,2) and (3,4).

Growth Pairs with 2 Pentagons

G2.12.1.1, $|V| = 12$ G2.12.1.2, $|V| = 14$ G2.16.1.1, $|V| = 16$ G2.16.1.2, $|V| = 20$ G2.16.2.1, $|V| = 16$ G2.16.2.2, $|V| = 18$ G2.16.2.3, $|V| = 20$ G2.16.3.1, $|V| = 16$

G2.16.3.2, $|V| = 20$ G2.20.1.1, $|V| = 20$ G2.20.1.2, $|V| = 24$ G2.20.2.1, $|V| = 20$ G2.20.2.2, $|V| = 26$ G2.20.2.3, $|V| = 28$ G2.20.3.1, $|V| = 20$ G2.20.3.2, $|V| = 22$

G2.20.3.3, $|V| = 26$ G2.20.3.4, $|V| = 26$ G2.20.4.1, $|V| = 20$ G2.20.4.2, $|V| = 26$ G2.20.4.3, $|V| = 26$ G2.20.5.1, $|V| = 20$ G2.20.5.2, $|V| = 24$ G2.20.5.3, $|V| = 26$

G2.20.5.4, $|V| = 28$ G2.20.6.1, $|V| = 20$ G2.20.6.2, $|V| = 26$ G2.20.7.1, $|V| = 22$ G2.20.7.2, $|V| = 26$ G2.20.8.1, $|V| = 20$ G2.20.8.2, $|V| = 26$ G2.20.8.3, $|V| = 28$

G2.20.8.4, $|V| = 30$ G2.22.1.1, $|V| = 23$ G2.22.1.2, $|V| = 25$ G2.22.2.1, $|V| = 23$ G2.22.2.2, $|V| = 25$ G2.22.3.1, $|V| = 23$ G2.22.3.2, $|V| = 27$ G2.24.1.1, $|V| = 24$

G2.24.1.2, $|V| = 28$ G2.24.1.3, $|V| = 32$ G2.24.2.1, $|V| = 24$ G2.24.2.2, $|V| = 32$ G2.24.3.1, $|V| = 24$ G2.24.3.2, $|V| = 30$ G2.24.3.3, $|V| = 32$ G2.24.3.4, $|V| = 34$

G2.24.4.1, $|V| = 24$ G2.24.4.2, $|V| = 28$ G2.24.4.3, $|V| = 30$ G2.24.4.4, $|V| = 32$ G2.24.5.1, $|V| = 24$ G2.24.5.2, $|V| = 30$ G2.24.5.3, $|V| = 34$ G2.24.6.1, $|V| = 24$

G2.24.6.2, $|V| = 34$ G2.24.7.1, $|V| = 24$ G2.24.7.2, $|V| = 32$ G2.24.7.3, $|V| = 36$ G2.24.7.4, $|V| = 36$ G2.24.8.1, $|V| = 24$ G2.24.8.2, $|V| = 26$ G2.24.8.3, $|V| = 32$

G2.24.8.4, $|V| = 32$ G2.24.8.5, $|V| = 34$ G2.24.8.6, $|V| = 36$ G2.24.9.1, $|V| = 24$ G2.24.9.2, $|V| = 32$ G2.24.9.3, $|V| = 32$ G2.24.9.4, $|V| = 34$ G2.24.9.5, $|V| = 36$

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G2.24.10.1, $|V| = 24$ G2.24.10.2, $|V| = 28$ G2.24.10.3, $|V| = 32$ G2.24.10.4, $|V| = 34$ G2.24.10.5, $|V| = 36$ G2.24.11.1, $|V| = 24$ G2.24.11.2, $V| = 32$ G2.24.11.3, $|V| = 34$

G2.24.11.4, $|V| = 36$ G2.24.12.1, $|V| = 24$ G2.24.12.2, $|V| = 28$ G2.24.12.3, $|V| = 32$ G2.24.12.4, $|V| = 32$ G2.24.12.5, $|V| = 34$ G2.24.12.6, $V| = 36$ G2.24.13.1, $|V = 24$

G2.24.13.2, $|V| - 30$ G2.24.13.3, $|V| - 32$ G2.24.13.4, $|V| - 36$ G2.24.13.5, $V| - 36$ G2.24.14.1, $|V| = 24$ G2.24.14.2, $|V| = 30$ G2.24.14.3, $|V| = 34$ G2.24.15.1, $|V| = 24$

G2.24.15.2, $|V| = 30$ G2.24.16.1, $|V| = 24$ G2.24.16.2, $|V| = 32$ G2.24.16.3, $|V| = 36$ G2.24.17.1, $|V| = 24$ G2.24.17.2, $|V| = 30$ G2.24.17.3, $|V| = 32$ G2.24.17.4, $|V| = 32$

G2.24.17.5, $|V| = 36$ G2.24.17.6, $|V| = 36$ G2.24.18.1, $|V| = 24$ G2.24.18.2, $|V| = 32$ G2.24.18.3, $|V| = 36$ G2.24.18.4, $|V| = 38$ G2.24.18.5, $|V| = 40$ G2.24.19.1, $|V| = 26$

G2.24.19.2, $|V| = 28$

Growth Pairs with 3 Pentagons

G3.15.1.1, $|V| = 15$ G3.15.1.2, $|V = 19$ G3.15.2.1, $|V| = 15$ G3.15.2.2, $|V| = 19$ G3.15.3.1, $|V| = 15$ G3.15.3.2, $|V| = 19$ G3.15.4.1, $|V| = 19$ G3.15.4.2, $|V| = 21$

G3.17.1.1, $|V| = 18$ G3.17.1.2, $|V| = 24$ G3.17.2.1, $|V| = 18$ G3.17.2.2, $|V| = 24$ G3.17.3.1, $|V| = 18$ G3.17.3.2, $|V| = 22$ G3.17.3.3, $|V| = 24$ G3.17.4.1, $|V| = 18$

G3.17.4.2, $|V| = 24$ G3.17.5.1, $|V| = 18$ G3.17.5.2, $|V| = 26$ G3.17.6.1, $|V| = 20$ G3.17.6.2, $V| = 24$ G3.19.1.1, $|V = 19$ G3.19.1.2, $|V| = 25$ G3.19.2.1, $|V| = 19$

G3.19.2.2, $|V| = 27$ G3.19.3.1, $|V| = 21$ G3.19.3.2, $|V| = 25$ G3.19.4.1, $|V| = 19$ G3.19.4.2, $|V| = 21$ G3.19.4.3, $|V| = 23$ G3.19.4.4, $|V| = 25$ G3.19.5.1, $|V| = 19$

G3.19.5.2, $|V| = 25$ G3.19.5.3, $|V| = 25$ G3.19.5.4, $|V| = 27$ G3.19.6.1, $|V| = 19$ G3.19.6.2, $|V| = 25$ G3.19.7.1, $|V| = 19$ G3.19.7.2, $|V| = 25$ G3.19.8.1, $|V| = 19$

G3.19.8.2, $|V| = 23$ G3.19.8.3, $|V| = 25$ G3.19.8.4, $|V| = 25$ G3.19.8.5, $|V| = 27$ G3.19.9.1, $|V| = 19$ G3.19.9.2, $|V| = 25$ G3.19.9.3, $|V| = 25$ G3.19.9.4, $|V| = 27$

G3.19.10.1, $|V| = 19$ G3.19.10.2, $|V| = 23$ G3.19.10.3, $|V| = 27$ G3.19.11.1, $|V| = 19$ G3.19.11.2, $|V| = 25$ G3.19.11.3, $|V| = 27$ G3.19.12.1, $|V| = 21$ G3.19.12.2, $|V| = 25$

G3.19.13.1, $|V| = 19$ G3.19.13.2, $|V| = 25$ G3.19.13.3, $|V| = 27$ G3.19.13.4, $|V| = 27$ G3.19.13.5, $|V| = 29$ G3.19.14.1, $|V| = 19$ G3.19.14.2, $|V| = 25$ G3.19.14.3, $|V| = 25$

G3.19.14.4, $|V| = 29$ G3.19.15.1, $|V| = 21$ G3.19.15.2, $|V| = 25$ G3.19.16.1, $|V| = 21$ G3.19.16.2, $|V| = 27$ G3.19.17.1, $|V| = 19$ G3.19.17.2, $|V| = 25$ G3.19.17.3, $|V| = 27$

G3.19.18.1, $|V| = 21$ G3.19.18.2, $|V| = 23$ G3.19.19.1, $|V| = 23$ G3.19.19.2, $|V| = 25$

Growth Pairs with 4 Pentagons

G4.14.1.1, $|V| = 14$ G4.14.1.2, $|V| = 18$ G4.14.2.1, $|V| = 16$ G4.14.2.2, $|V| = 22$ G4.14.3.1, $|V| = 18$ G4.14.3.2, $|V| = 22$ G4.16.1.1, $|V| = 17$

G4.16.1.2, $|V| = 23$ G4.16.2.1, $|V| = 17$ G4.16.2.2, $|V| = 25$ G4.16.3.1, $|V| = 17$ G4.16.3.2, $|V| = 23$ G4.16.4.1, $|V| = 17$ G4.16.4.2, $|V| = 23$

G4.16.4.3, $|V| = 25$ G4.16.5.1, $|V| = 17$ G4.16.5.2, $|V| = 25$ G4.16.6.1, $|V| = 19$ G4.16.6.2, $|V| = 23$ G4.16.7.1, $|V| = 21$ G4.16.7.2, $|V| = 23$

Chart 1

Growth Pairs with 5 Pentagons

G5.15.1.1, $|V| = 16$ G5.15.1.2, $|V| = 24$ G5.15.2.1, $|V| = 18$ G5.15.2.2, $|V| = 30$ G5.15.3.1, $|V| = 16$ G5.15.3.2, $|V| = 22$ G5.15.4.1, $|V| = 18$

G5.15.4.2, $|V| = 30$ G5.15.5.1, $|V| = 18$ G5.15.5.2, $|V| = 28$ G5.15.5.3, $|V| = 30$ G5.15.5.4, $|V| = 34$ G5.15.6.1, $|V| = 20$ G5.15.6.2, $|V| = 28$

p pentagons and boundary length l that has the bth boundary listed for given p and l and is the nth patch for given p, l, b is indexed G$p.l.b.n$. The growth pairs are all pairs (G$p.l.b$.1,G$p.l.b.n$) with $n > 1$ for which a patch G$p.l.b.n$ exists. The catalogue shows the numbers of vertices in each patch, from which it is easy to identify the processes that add 2, 4, ... atoms to the fullerene.

In the range of examples presented in the catalogue it is always possible to find for the given boundary at least one patch P such that all irreducible pairs contain P. This simplifies the presentation of the results and gives rise to the format described above. However, this is not a general property, and the format would need modification if the range of the catalogue were to be extended. Figure 5 shows an example of a set of four patches that fall into two pairs with no common patch.

Whereas for two pentagons most of the pairs in the catalogue have isolated pentagons and therefore are energetically preferrable in the sense mentioned before, for three pentagons the fraction is much smaller due to the restriction to small patches. For four or five pentagons the patches we list are simply too small to allow the pentagons to be isolated. For larger values of the boundary length and therefore larger patches, isolated pentagon pairs do of course exist.

Although space considerations restrict the catalogue to small examples, some infinite series can evidently be constructed from pairs that occur in the list. Generalizations of the Endo−Kroto pair (G2.12.1.1, G2.12.1.2), for example, are as follows: the pairs (G2.12.1.1, G2.12.1.2), (G2.16.3.1, G2.16.3.2), (G2.20.8.1.1, G2.20.8.1.2), and (G2.24.18.1, G2.24.18.2) are the first four entries of an infinite series of pairs for boundary lengths $b = 4n$, $n \geq 3$ that increase the number of atoms by $2n - 4$; the pairs (G2.12.1.1, G2.12.1.2), (G2.16.2.1, G2.16.2.2), (G2.20.3.1, G2.20.3.2), and (G2.24.8.1, G2.24.8.2) are the first four entries of an infinite series of pairs for boundary lengths $b = 4n$, $n \geq 3$ that increase the number of atoms by 2. There are also sequences that do not start with the Endo−Kroto pair, as e.g. (G2.16.1.1, G2.16.1.2), (G2.20.2.1, G2.20.2.2), and (G2.24.7.1, G2.24.7.2), and there are certainly other sequences where the rule for extending the series is harder to see.

Since for three or more pentagons the number of pairs grows very rapidly, we were able to list the pairs only for very small values of the boundary length. For this reason it is harder to detect an infinite series with large numbers of

pentagons, as only the first one or two entries would fall within the limits of the table. Nevertheless, the pairs (G3.15.3.1, G3.15.3.2) and (G3.19.17.1, G3.19.17.2) are examples where it is easy to see the structure of the infinite sequence starting with these pairs.

REFERENCES AND NOTES

(1) Grünbaum, B.; Motzkin, T. The number of hexagons and the simplicity of geodesics on certain polyhedra. *Can. J. Math.* **1963**, *15*, 744−751.

(2) Fowler, P. W.; Manolopoulos, D. E. *An atlas of fullerenes*; Oxford University Press: Oxford, 1995.

(3) Stone, A. J.; Wales, D. J. Theoretical studies of icosahedral C_{60} and some related species. *Chem. Phys. Lett.* **1986**, *128*, 501−503.

(4) Endo, M.; Kroto, H. W. Formation of carbon nanofibers. *J. Phys. Chem.* **1992**, *96*, 6941−6944.

(5) Heath, J. R. Synthesis of C_{60} from small carbon clusters: a model based on experiment and theory. In *Fullerenes: Synthesis, Properties and Chemistry of Large Carbon Clusters*; Hammond, G. S., Kuck, V. J., Eds.; ACS Symposium Series no. 481; American Chemical Society: Washington, DC, 1991; pp 1−23.

(6) O'Brien, S. C.; Heath, J. R.; Curl, R. F.; Smalley, R. E. Photophysics of buckminsterfullerene and other carbon cluster ions. *J. Phys. Chem.* **1988**, *88*, 220−230.

(7) Brinkmann, G.; Fowler, P. W.; Justus, C. A catalogue of isomerisation transformations of fullerene polyhedra. *J. Chem. Inf. Comput. Sci.* **2003**, *43*, 917−927.

(8) Astakhova, T. Y.; Vinogradov, G. A. New isomerisation operations for fullerene graphs. *J. Mol. Struct. (THEOCHEM)* **1998**, *430*, 259−268.

(9) Babic, D.; Trinajstic, N. Planar rearrangements of fullerenes *J. Mol. Graphics Model.* **2001**, *19*, 210−215.

(10) Manolopoulos, D. E.; Fowler, P. W. Downhill on the fullerene road: a mechanism for the formation of C_{60}. In *The chemical physics of the fullerenes 10 (and 5) years later;* Andreoni, W., Ed.; Kluwer Academic Press: Dordrecht, 1996; pp 51−69.

(11) Curl, R. F. On the formation of fullerenes. *Philos. Trans. R. Soc. London Ser. A* **1993**, *343*, 19−32.

(12) Sah, C. H. Combinatorial Construction of Fullerene Structures. *Croat. Chem. Acta* **1993**, *66*, 1−12.

(13) Bornhöft, J.; Brinkmann, G.; Greinus, J. Pentagon-hexagon-patches with short boundaries. *Eur. J. Combinatorics* **2003**, *24*, 517−529.

(14) Greinus, J. Patches mit minimaler Randlänge. Diplomarbeit, Bielefeld, 2001.

(15) Brinkmann, G.; Delgado Friedrichs, O.; Dress, A.; Harmuth, T. Cage − a virtual environment for studying some special classes of large molecules. *Match* **1997**, 36, 233−237. See http://www.mathematik.uni-bielefeld.de/∼CaGe.

(16) Guo, X.; Hansen, P.; Zheng, M. Boundary uniqueness of helicenes. *Discrete Appl. Mathematics* **2002**, *118* (3), 209−222.

(17) Brinkmann, G.; Delgado Friedrichs, O.; von Nathusius, U. Numbers of faces and boundary encodings of patches. Submitted for publication.

(18) Brinkmann, G.; Justus, C. Numbers of Faces in Disordered Patches. Manuscript in preparation.