

# A Catalogue of Isomerization Transformations of Fullerene Polyhedra

G. Brinkmann, P. W. Fowler,\* and C. Justus

Fakultät für Mathematik, Universität Bielefeld, D 33501 Bielefeld, Germany, School of Chemistry, University of Exeter, Exeter, EX4 4QD United Kingdom, and Fakultät für Mathematik, Universität Bielefeld, D 33501 Bielefeld, Germany

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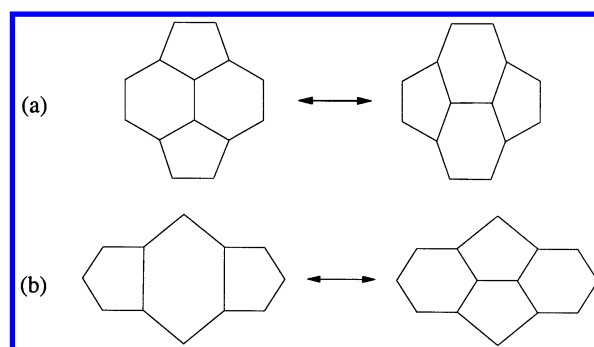
Representation of isomerization and carbon insertion or extrusion mechanisms as patch replacements on a fullerene surface allows construction of a catalogue of topologically distinct local transformations of fullerenes, classified by patch boundary and pentagon content. All isomerization patches and isomerization pairs containing up to five pentagons and with an upper limit for the boundary length depending on the number of pentagons are listed. Several infinite series of transformations are identified.

## INTRODUCTION

Fullerenes are polyhedral carbon cages in which each atom is directly bonded to three neighbors and each face of the polyhedron is either a pentagon or a hexagon. A fullerene  $C_n$  has 12 pentagonal and  $(n/2 - 10)$  hexagonal rings and typically has a large variety of mathematically possible isomers which differ in the mutual arrangement of the pentagons.

Transformations of one isomeric fullerene polyhedron to another with the same number of vertices or to one that differs (by an even number) in vertex count are not only of mathematical interest in construction and description of the polyhedra but also have direct relevance to the chemistry and physics of the molecules. For example, it is observed that the experimentally characterized fullerenes are generally found among those predicted to have low total energy within their isomer set, suggesting a possible role for annealing processes converting less to more stable isomers. Likewise, the mass-spectral signature of the products of graphite vaporization and laser-induced “shrink-wrapping” experiments support the hypothesis of inflation and deflation of fullerenes by  $C_2$  gain and loss.<sup>6</sup>

Two simple proposals for mechanisms of annealing and  $C_2$  insertion were made soon after the discovery of fullerenes: the Stone–Wales isomerization<sup>7</sup> and the Endo–Kroto  $C_2$  insertion,<sup>8</sup> respectively. Taken as purely topological descriptions of interconversion processes, they can be used as the basis of a “fullerene road”<sup>9,10</sup> that connects the smallest fullerenes with hexagonal rings to the abundant  $C_{60}$  and  $C_{70}$  species and for construction of isomerization/growth maps that link isomers into families. Detailed quantum mechanical scrutiny confirms the high activation barriers expected when Figure 1 is taken as a literal description of concerted atom movements but suggests topologically equivalent pathways with substantially lower barriers.<sup>12,13</sup> Generalizations to rearrangements that involve larger portions of the fullerene surface, or insertion/extrusion of larger  $C_{2m}$  fragments, have also been proposed<sup>14–19</sup> and in some cases tested against quantum calculations. As these proposals have proliferated,



**Figure 1.** The two simplest mechanisms for interconversion of fullerene polyhedra: (a) the Stone–Wales isomerization<sup>7</sup> and (b) the Endo–Kroto  $C_2$  insertion.<sup>8</sup>

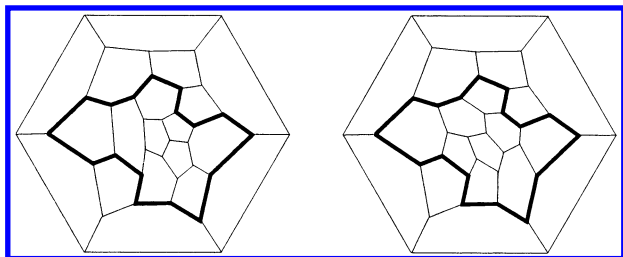
the increasing need for a systematic treatment has been noted by several authors.<sup>16,17</sup>

The aim of the present work is to consider a unified framework that allows construction and cataloging of the distinct topological possibilities for isomerization/growth processes. The focus is specifically on the identification and enumeration of the mathematically possible local transformations of fullerenes, rather than on their mechanistic realization and physical energetics. An explicit list of isomerization processes involving up to five pentagons and taking place within patches up to a specified boundary size is given at the end of the paper. It is hoped that construction of the catalogue will serve as a firm basis for further quantum mechanical study of these important aspects. Step-by-step consideration of possibilities already reveals classes of transformations of fullerene polyhedra that have escaped attention in the existing literature.

## PRELIMINARIES

The basic object in the present approach to the classification of local fullerene transformations is the *patch*. The idea is that, since the transformation is “local”, the surface of the fullerene polyhedron can be partitioned into two parts by a closed *boundary circuit* of vertices and edges, drawn such that all changes are confined to the interior of the disc-like region it encloses. Each vertex in the boundary is incident

\* Corresponding author e-mail: PWFowler@exeter.ac.uk.



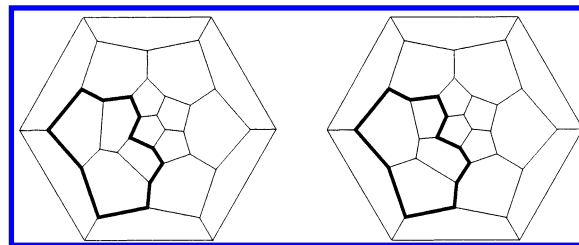
**Figure 2.** A cut and paste operation with an isomerization pair that leads to an isomorphic fullerene. This is the isomer 36:7 of  $C_{36}$  in the notation of ref 6.

with two edges lying in the boundary and one edge that points into either the interior or exterior region. If these possibilities are represented by 1 and 0, respectively, boundaries can be labeled with lexicographic binary codes. The boundary and all interior edges and vertices constitute the patch. A transformation can be imagined as a formal cut-and-paste operation, in which the fullerene is cut along the boundary, the whole patch is lifted out and is replaced by another that “fits” the same boundary (in the sense of having the same boundary code). The replacing patch may be (i) a rotated or reflected copy of the original, (ii) a nonisomorphic patch with the same number of vertices and edges as the original, or (iii) a (necessarily nonisomorphic) patch with a different number of vertices. The first two possibilities refer to isomerizations and the third to inflation or deflation of the fullerene, in which case the change in vertex count must be an even number since initial and final polyhedra are to remain trivalent. We can refer to an *isomerization patch* in case (i), an *isomerization pair* in case (ii), and an *inflation patch* in case (iii).

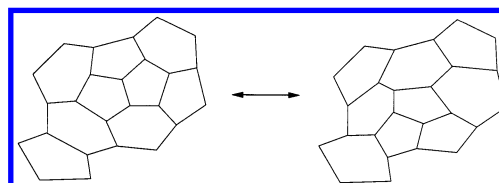
This picture is clearly a combinatorial rather than an affine description of the transformation; in physical reality, the molecular polyhedron will typically be subject to geometric relaxation, both within and beyond the boundary of the patch, as the structure changes to accommodate the new arrangement of vertices and edges.

When will such a cut-and-paste operation lead to a product that is different from the starting isomer? The product and starting isomers will obviously be distinct in the cases of inflation pairs. In case of isomerization pairs, the product and starting isomer will generally differ but not always. See Figure 2 for an example.

The requirement that the patch boundary, but not the whole fullerene, should “look the same” before and after the transformation can be translated into a precise symmetry restriction. A *necessary* condition for an isomerization patch to give a different product is that the boundary should possess a larger automorphism group than the patch or its complement in the fullerene; the original and replaced versions of the patch are then related by an automorphism of the boundary that is not an automorphism of any of the parts. In more chemical language, the automorphism group would be called the “topological” or “maximum” site point group, i.e., the point symmetry group of the object if embedded in its most symmetrical way on a spherical cap. The site group of the patch is  $C_{mv}$  or a subgroup, with  $m = 6, 5, 3$ , or 2 if the patch belongs to a fullerene. For the symmetry group of the boundary, other values for  $m$  are also possible. For example (Figure 1), the Stone–Wales patch has boundary code (100)<sup>4</sup> which has automorphism group  $C_{4v}$ , whereas



**Figure 3.** A Stone–Wales transformation that converts a fullerene into a copy of itself. The fullerene is an isomer of  $C_{34}$  (34:2 in the notation of ref 6).



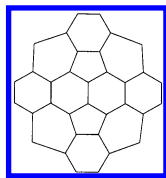
**Figure 4.** Isomerization via exchange of a pair of nonisomorphic patches with identical boundary codes.

the patch with all its internal structure included has only  $C_{2v}$ ; conversion of the Stone–Wales patch to its replacement (Figure 1(a)) is achieved by a  $C_4$  rotation of the interior within a fixed boundary;  $C_4$  is present in the boundary automorphism group  $C_{4v}$  but not in  $C_{2v}$ .

Note that this condition on boundary and patch groups is not *sufficient* to ensure that the product fullerene is distinct from the original; an example where this is not the case is given in Figure 3. Cases where a Stone–Wales transformation interconverts enantiomeric fullerenes, and hence produces isomorphic graphs but with distinct spatial embeddings, are common, with the smallest example being the  $D_2$  symmetric isomer 1 of  $C_{28}$ , which is both the smallest fullerene that has a Stone–Wales patch and the smallest chiral fullerene.

The present “patchwork” approach has some similarities with a method for generation of isomerization transformations defined previously by Astakhova and Vinogradov.<sup>16</sup> In their approach, a transformation is defined by a central patch and a circumscribing “hoop” of faces which separates the patch from the remainder of the fullerene. In the transformation, all connections from the main part of the fullerene across the hoop to the central patch are broken, the central patch is either rotated or reflected, and new connections remade across the hoop region to recover a fullerene graph. The net effect may be of type (i) (isomerization patch) or type (ii) (isomerization pair) in the present classification, but the transformations defined in Astrakhova and Vinogradov’s paper<sup>16</sup> do not cover the whole spectrum of possibilities. The two approaches both define two regions of the fullerene that have unchanging internal structures but differ in that our patch+complement constitute the whole fullerene, whereas the patch in ref 16 is isolated from the rest of the fullerene by a zone that has a variable structure.

The Stone–Wales transformation is one example of an isomerization patch which can be described in the cut-and-paste analogy as achieved by making a different gluing of the same patch. However, *any* two patches with the same boundary code and vertex number form an isomerization pair. Figure 4 shows the smallest such example for patches with five or fewer pentagons, and others are listed in the main



**Figure 5.** A circumscribed Stone–Wales patch.

catalogue (see below). Patches of this kind would fall outside the classification proposed by Astakhova and Vinogradov.

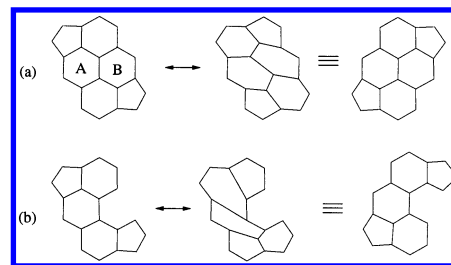
In constructing a catalogue, several potential problems arise and must be solved by making appropriate technical definitions. If the construction of patches were allowed to range without restriction over all possible simply connected groups of pentagons and hexagons, a given transformation could appear many times in superficially different guises. For example, the Stone–Wales patch (Figure 1(a)), its circumscription with 1 layer of hexagons (Figure 5), or with larger numbers of rings 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 patch*. An isomerization patch is called *irreducible* if there is an automorphism of the boundary that is not an automorphism of the patch and that does not map any *removable* face onto another removable face of the same size. A removable face is a face 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.

In cases (ii) and (iii) the definition of reducibility is similar. A pair of patches (either an isomerization pair or an inflation pair) is irreducible if there is an *isomorphism* that maps the boundary of one member of the pair to the boundary of the other with preservation of the vertex degrees and that does not map any removable face onto another removable face of the same size.

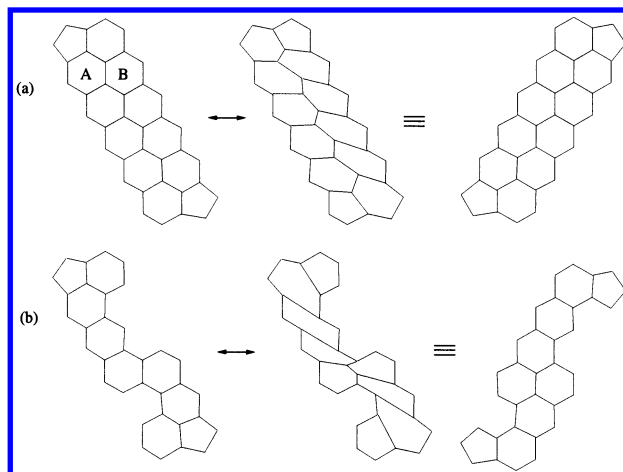
Note that, under this definition, unions of irreducible pairs or patches can occur as larger irreducible pairs or patches.

In the following, the term *nonunique* boundary will be used for a boundary cycle that occurs as the boundary cycle of at least one irreducible pair or *irreducible patch*.

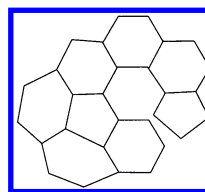
To give an order to the catalogue, that goes from “small” to “large” transformations, it is necessary to adopt a criterion of size. Here the irreducible patches and pairs are separated into classes according to the number of pentagons they contain and then ordered by boundary length and number of vertices. As noted earlier, reduction of a patch may actually increase its boundary length. Reduction may also affect the representation of a particular “physical” isomerization as a patch or as a pair. Thus, the “long Stone–Wales” or generalized pyracylene transformation shown in Figure 6<sup>15,18</sup> can be drawn as a parallelogram-like patch that leads from parent to product by a reflection symmetry of the boundary (Figure 6a). However this patch is reducible, by the definition, as there is an automorphism (a reflection in the group  $C_{2v}$ ) of the boundary, not present in the  $C_2$  group of the patch, that exchanges the central hexagons A and B, each of which is individually removable without causing disconnection of the patch. The entry in the catalogue will instead be the irreducible isomerization patch shown in



**Figure 6.** A “long Stone–Wales” transformation represented as (a) a reducible isomerization patch and (b) as an irreducible isomerization patch.



**Figure 7.** A “long Stone–Wales” transformation represented as (a) a reducible isomerization patch and (b) as one of the corresponding irreducible isomerization pairs.



**Figure 8.** An irreducible isomerization patch that is not embeddable in a classical pentagon/hexagon fullerene.

Figure 6b. The other “long Stone–Wales” transformation shown in Figure 7 is reducible in more than one way. One of the entries in the catalogue will be the irreducible isomerization pair shown in Figure 7b.

A similar argument would apply to the generalized Stone–Wales transformation in which rings A and B are both pentagons; the catalogue entry would be an isomerization pair of patches each containing three pentagons, rather than the  $C_{2h}$  symmetric single patch.

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 patch such as the one shown in Figure 8, 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. Embeddability is easily decided by inspection in small cases, but to check that some hidden non-local 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 less than 60 vertices. Those patches or pairs that were not found in fullerenes with up to 100 vertices could easily be shown not to be present in any fullerene, since they would require the

presence of a face of size at least 7. They were deleted from the catalogue list by hand.

### PROGRAM AND ALGORITHM

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 ref 4 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  $p$  we can determine the maximum and minimum numbers of C-atoms of a planar polycyclic hydrocarbon with this boundary length.

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 1) is started for that formula, and the output structures are examined for their symmetry group, their boundary encoding, and the symmetry group of their boundary encoding. If having been detected that the symmetry group of the boundary is richer than that of the patch, the structure is checked for reducibility and, if no possibility for a reduction is found, is output. At the same time, the boundary encoding is stored in order to be able to determine those encodings for which nonisomorphic structures 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 irreducible pairs are computed and output.

Unfortunately no independent results to check our programs 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 at the end of this article for which the group, 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.

Some theoretical results are available for  $p = 0$ . It is well known that any patch consisting solely of hexagons is either such that its interior is determined uniquely by its boundary, or it is not embeddable in the graphite sheet. In fact for  $p = 0$  every embedding of a patch that has no unique interior must cover at least one point three times when embedded in the graphite sheet.<sup>3</sup> Though patches with this overlapping property can occur in fullerenes, no fullerene patches with a nonunique interior of only hexagons or a richer symmetry group of the boundary than the interior are known. Our computer search confirmed that up to a boundary length of 46 no nonunique boundaries exist. For  $p = 0$  Guo, Hansen, and Zheng<sup>5</sup> have proved that the number of faces within a

boundary is determined uniquely by the boundary, and from this it follows that no inflation patches 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 is determined by the boundary.<sup>2</sup>

For  $p = 1$  it is an open question whether inflation patches do exist and whether patches with nonunique boundary can occur in fullerenes. Up to boundary length 41, no nonunique boundaries that can occur in fullerenes were found.

### THE PATCHWORK CATALOGUE

The result of our systematic "patchwork" approach to isomerization transformations of fullerenes is an ordered catalogue of isomerization patches and isomerization pairs, to the best of our knowledge complete up to the stated limits on boundary size and number of nonspectator pentagons involved. Cases with 2–5 pentagons are listed explicitly, ordered by boundary length and then lexicographically by boundary code. For space reasons, the list is truncated at boundary lengths (patches): 34 (2 pentagons), 27 (3 pentagons), 24 (4 pentagons), 25 (5 pentagons); (pairs) 32 (2 pentagons), 25 (3 pentagons), 22 (4 pentagons), 19 (5 pentagons). Each entry in the catalogue consists of a drawing or pair of drawings and a caption. The captions of the figures of *isomerization patches* give first the boundary encoding of the patch and in brackets the length of the boundary, the number of atoms, the size of the automorphism group of the boundary, and the size of the automorphism group of the patch in this order. The captions of the figures of *isomerization pairs* give the boundary encoding of the patches, the length of the boundary, and the number of atoms, in this order. Each entry in the patch list is given a label **I** $x$ : $y$ , and each pair in the pairs list is given a label **II** $x$ : $y$ , where  $x$  is the number of pentagons and  $y$  the position in the list of cases with fixed  $x$ . The labels are in the lower right corners of the figures.

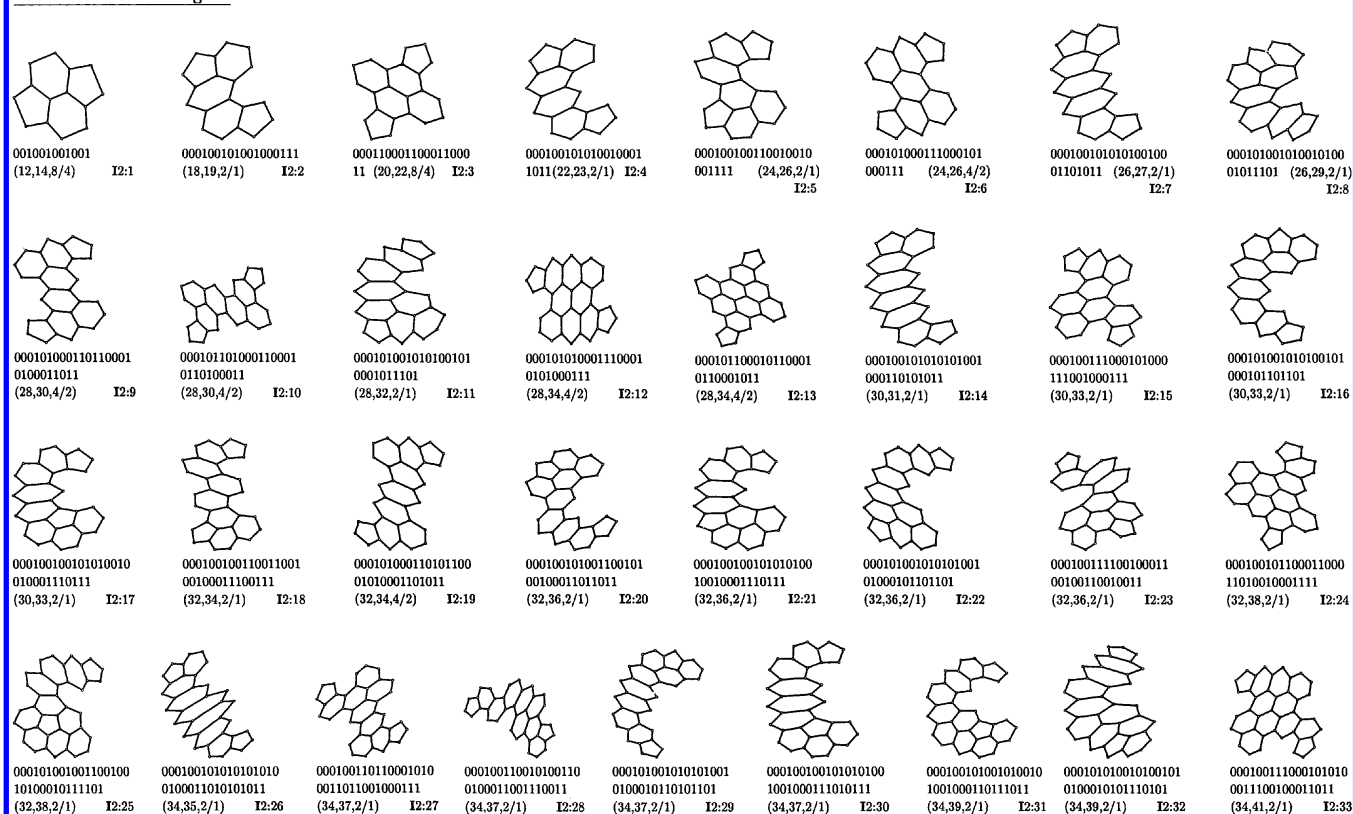
The first part of the catalogue, the list of isomerization patches, contains as it must, a number of previously identified isomerization transformations. First in order, as smallest in boundary length and involving fewest pentagons, is the Stone–Wales or pyracylene transformation, **I**2:1, which was also historically the first fullerene transformation to be proposed. This notation patch has a boundary of length 12, enclosing two vertices and its boundary cycle considered as a circuit on a sphere, has a 4-fold rotational axis lying at the junction of four reflection planes, whereas the boundary-plus-interior has only 2-fold rotational symmetry and two mirror planes. Hence its label is (12, 14, 8/4). Note that the boundary and patch symmetries,  $C_{4v}$  and  $C_{2v}$ , apply to the objects as caps on a sphere: the isolated objects have maximum symmetries  $D_{4h}$  and  $D_{2h}$ , with orders 16 and 8, respectively.

Next, **I**2:2 is the first of the generalizations of the Stone–Wales transformation. As noted above, this "long Stone–Wales patch" in which two faces separate the two pentagon–hexagon pairs within which pairwise exchange takes place, includes only five faces. The "bay" area bounded by the subsequence 01110 could be occupied by either a spectator hexagon or spectator pentagon when the patch is embedded in a fullerene. Representations in the literature include these



Chart 1

## Patches with 2 Pentagons



## Patches with 3 Pentagons

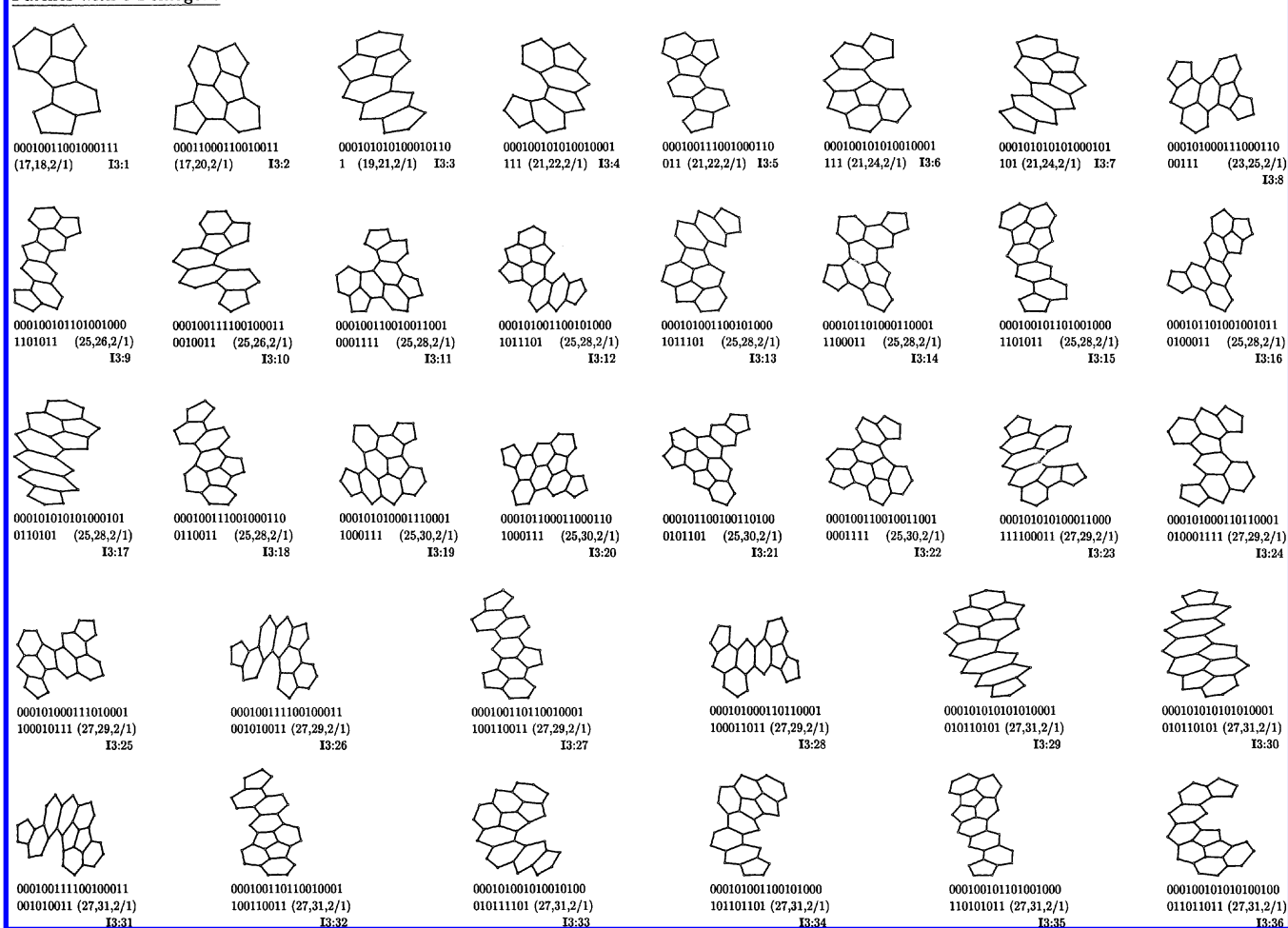
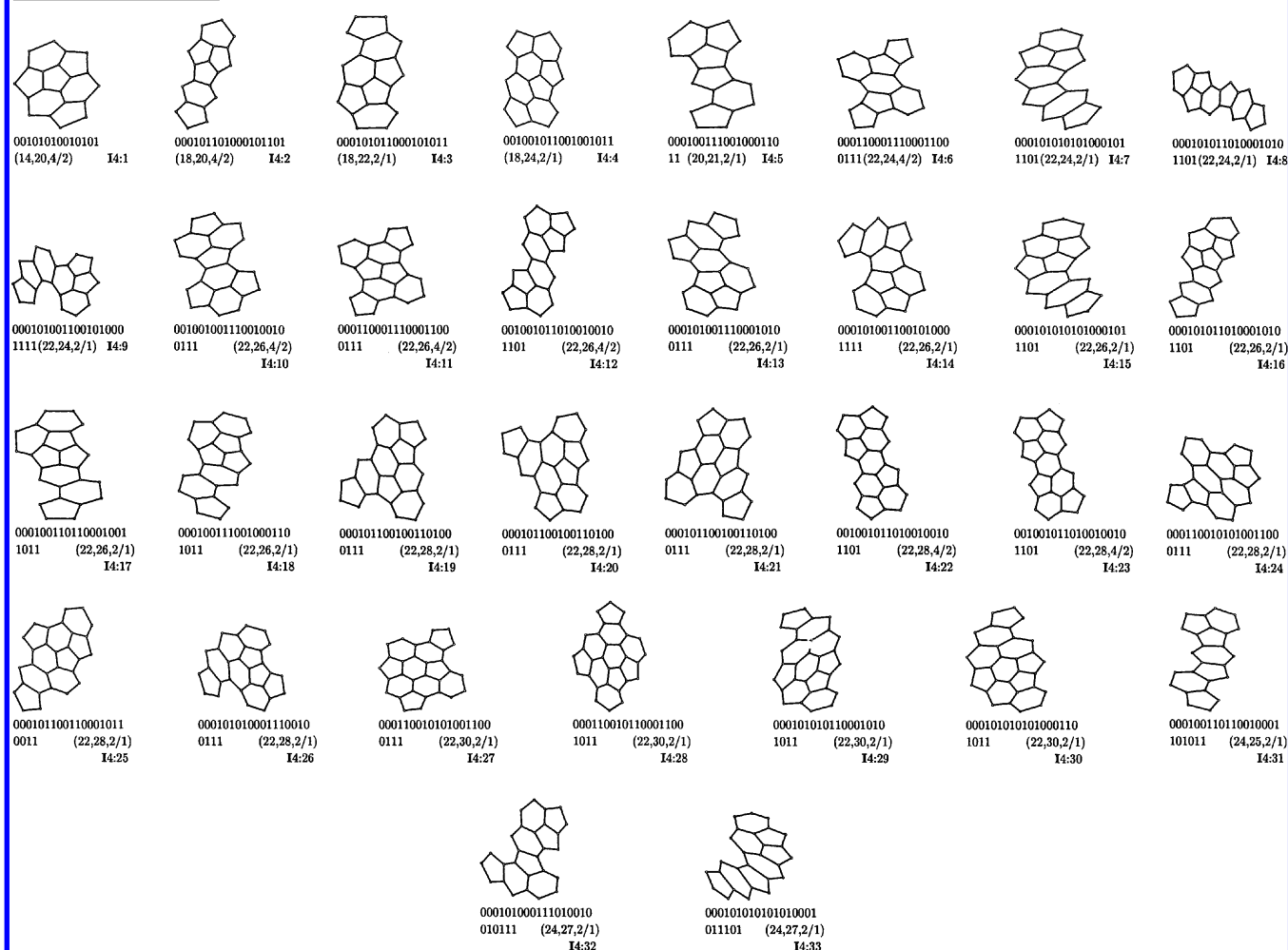


Chart 1. (Continued)

## Patches with 4 Pentagons



## Patches with 5 Pentagons

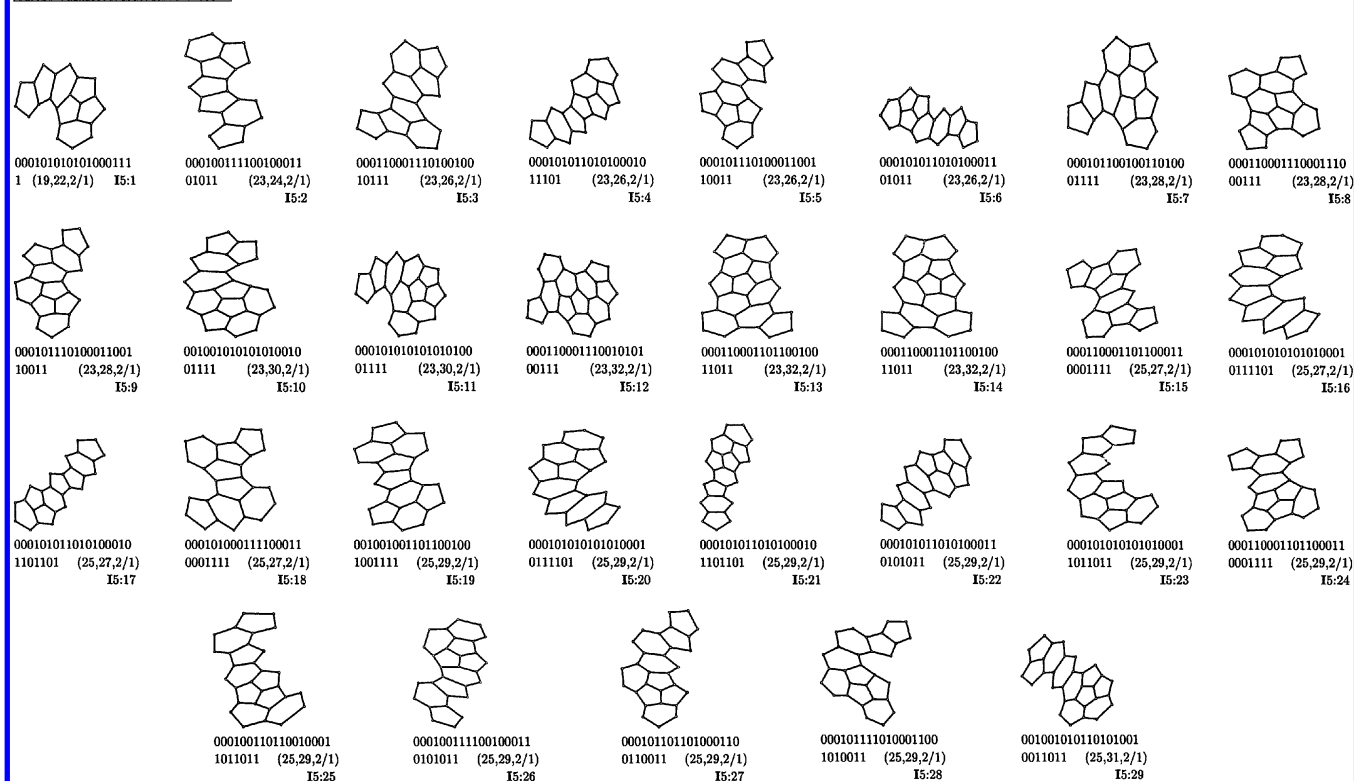


Chart 1. (Continued)

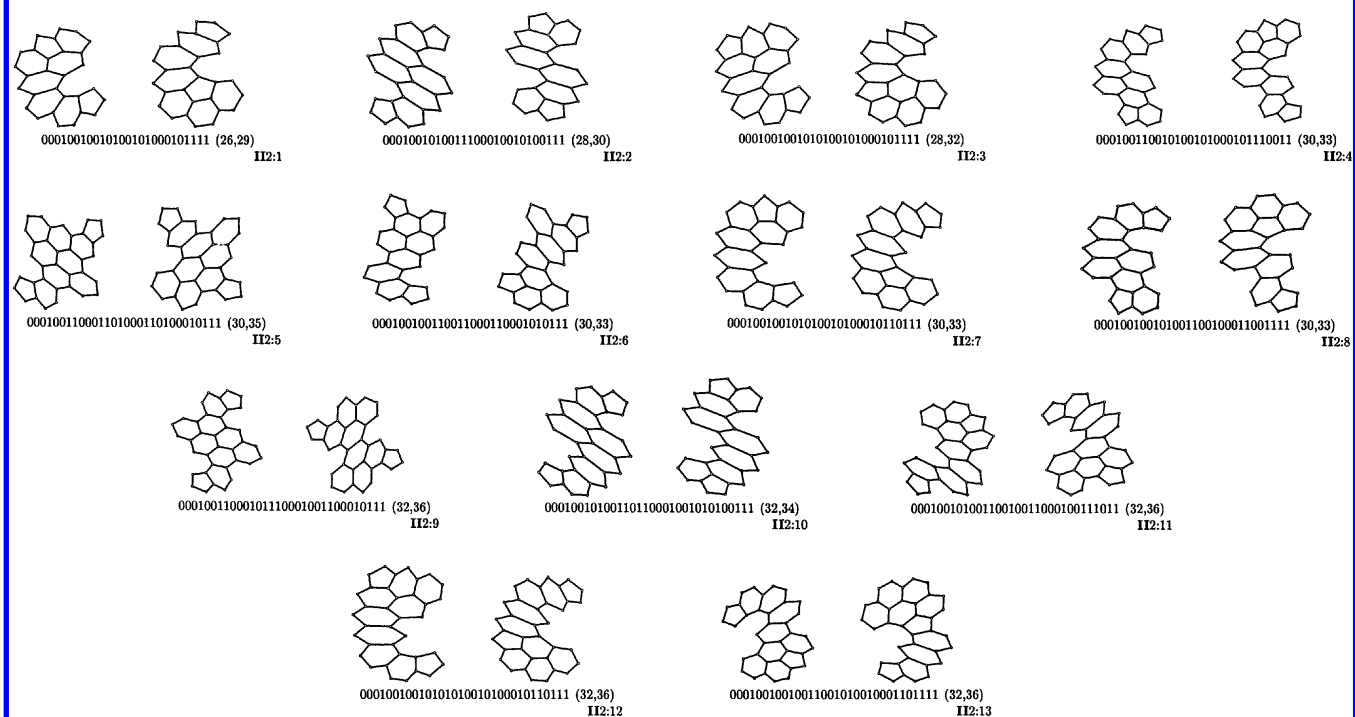
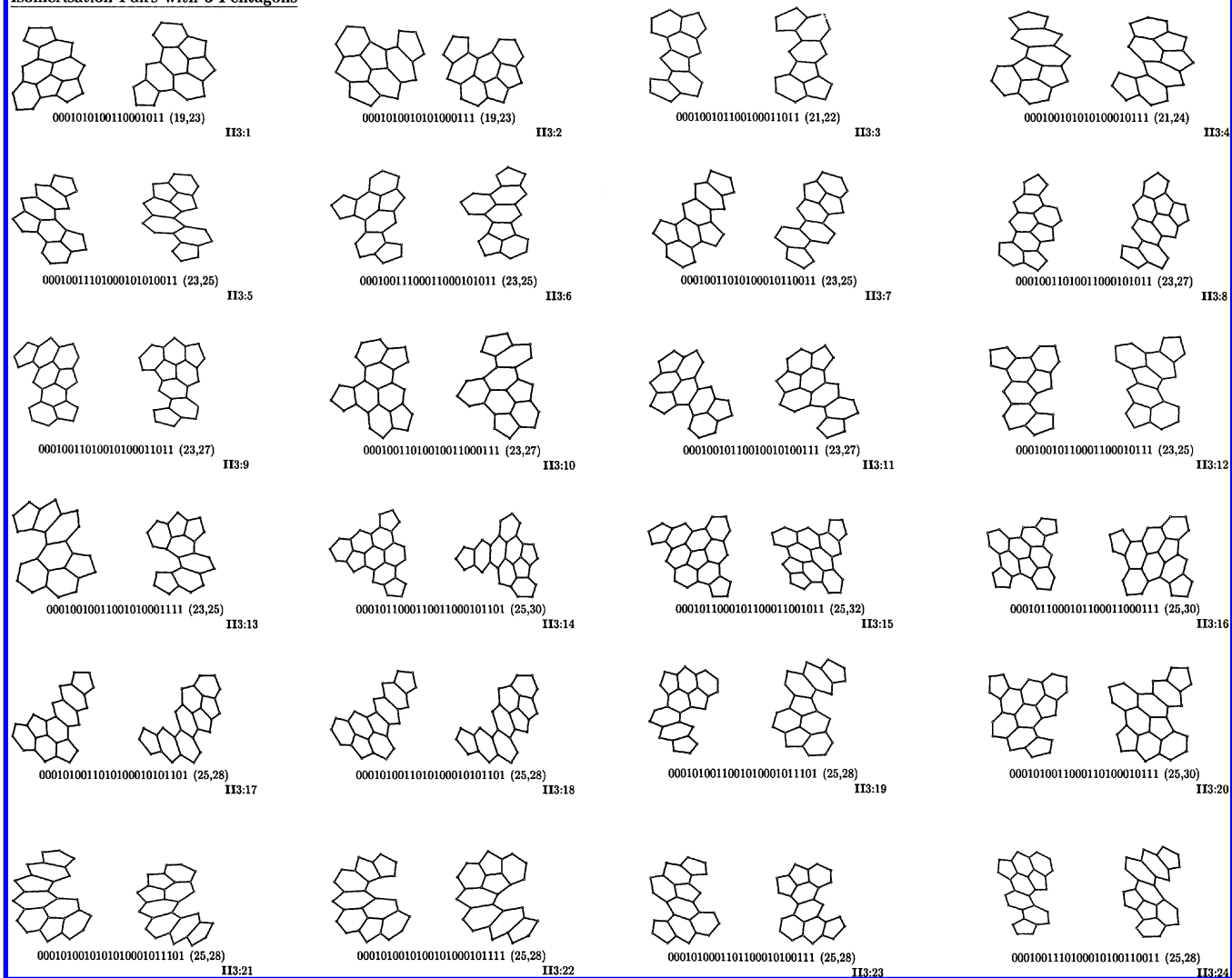
**Isomerisation Pairs with 2 Pentagons****Isomerisation Pairs with 3 Pentagons**

Chart 1. (Continued)

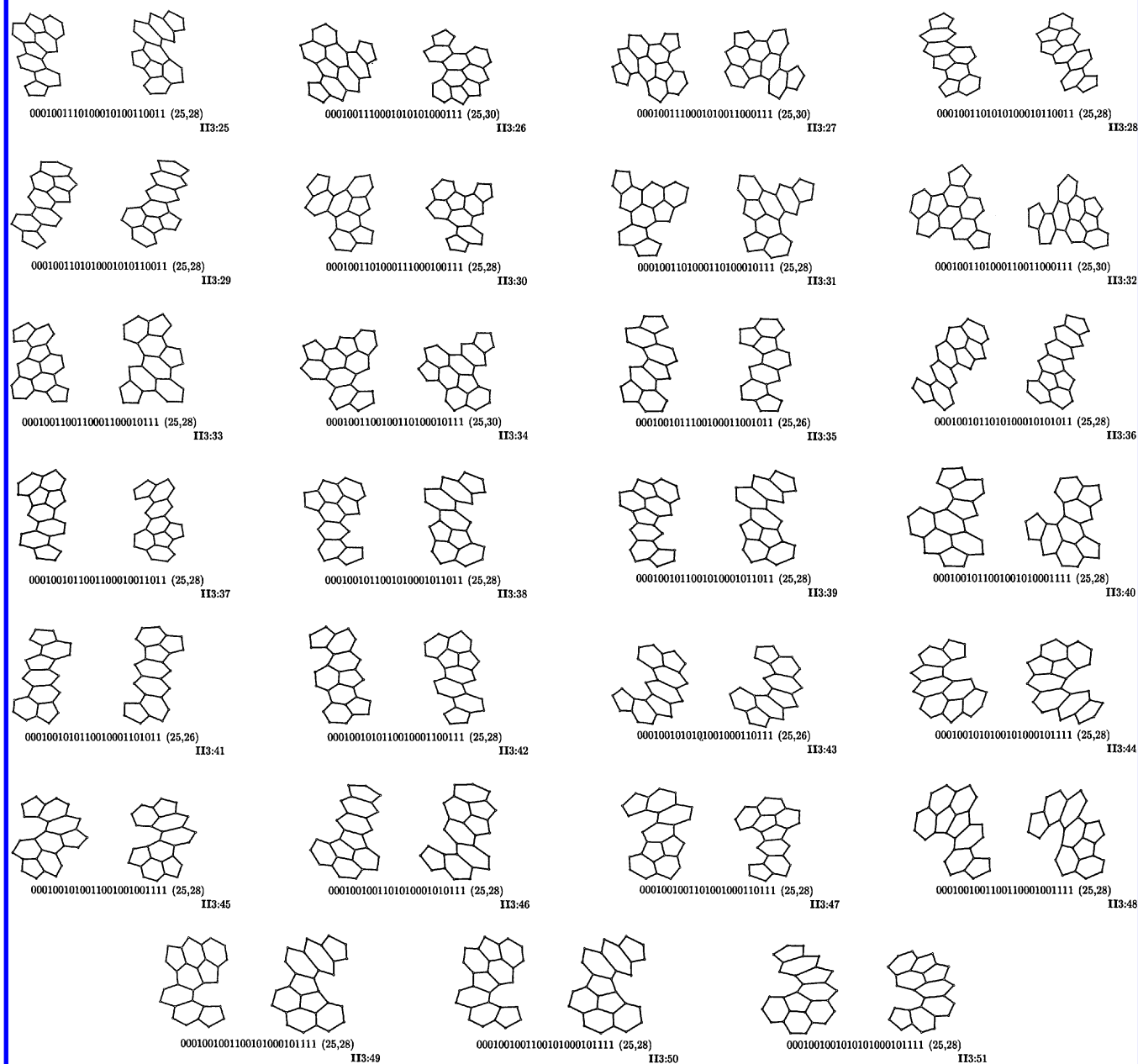
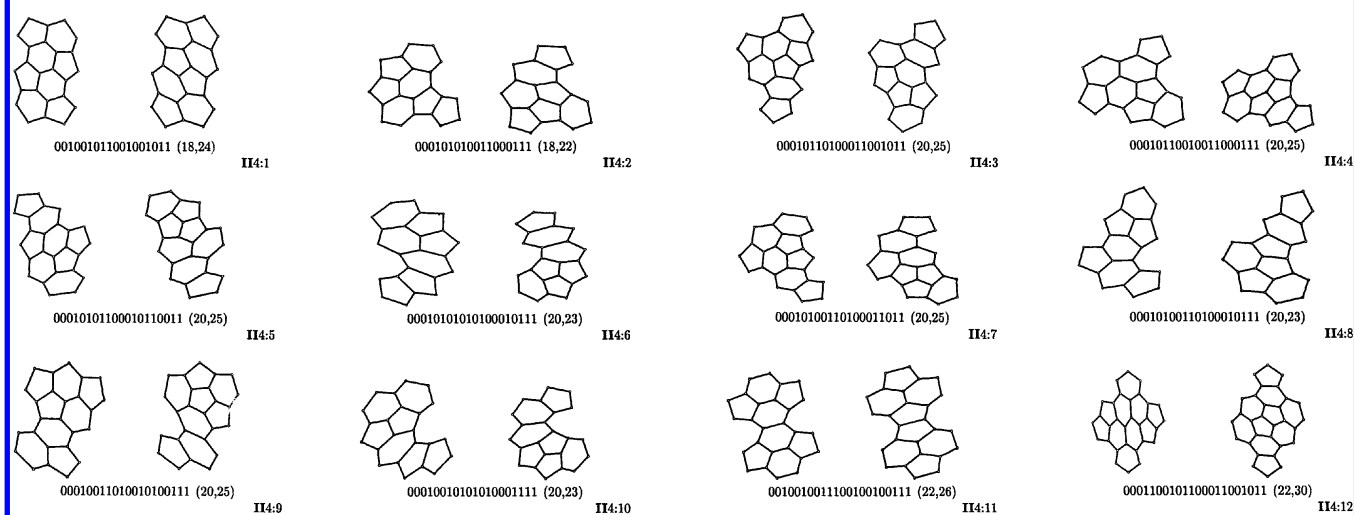
**Isomerisation Pairs with 3 Pentagons (Continued)****Isomerisation Pairs with 4 Pentagons**



Chart 1. (Continued)

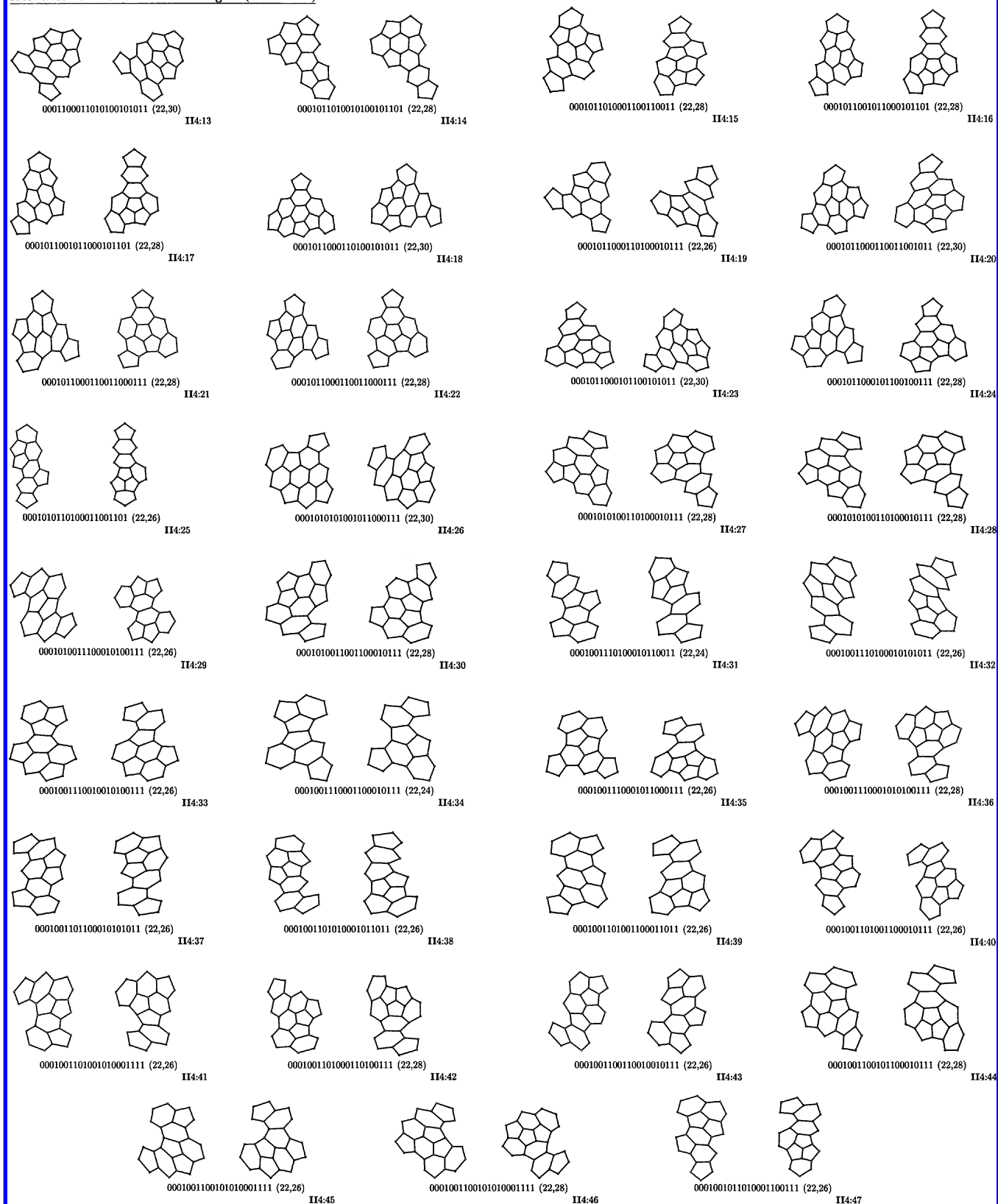
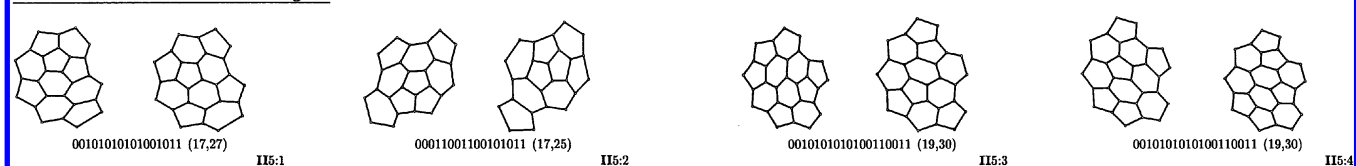
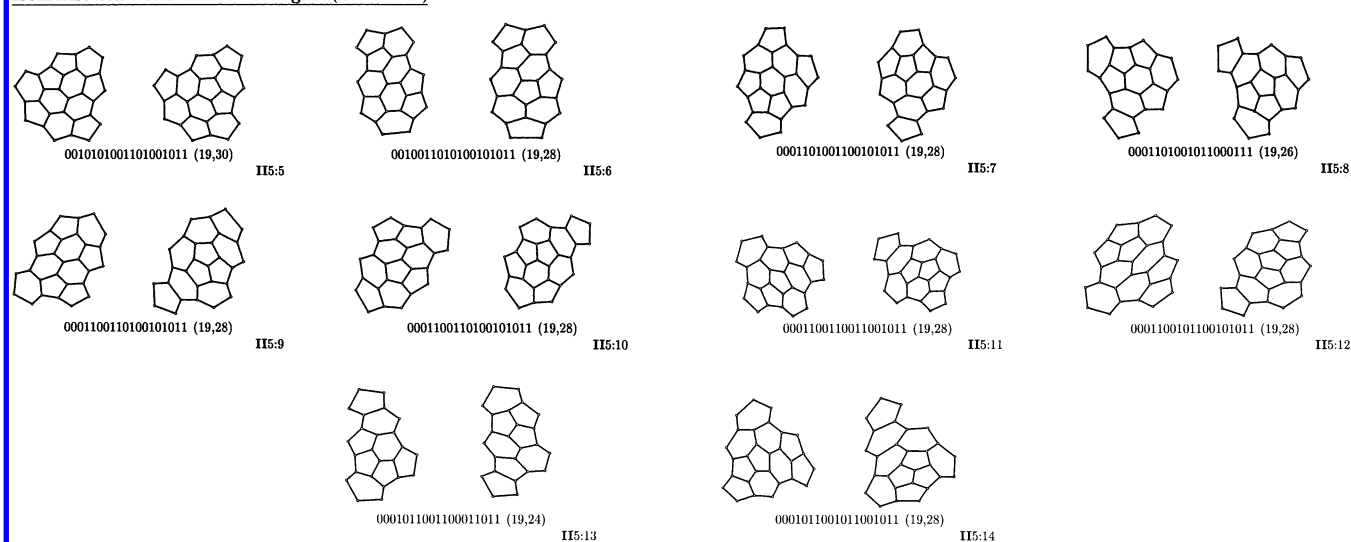
**Isomerisation Pairs with 4 Pentagons (Continued)****Isomerisation Pairs with 5 Pentagons**

Chart 1. (Continued)

## Isomerisation Pairs with 5 Pentagons (Continued)



removable faces, and previous authors would take the two fillings of the bay of **I2:2** as different transformations. In **I2:2** the bridging hexagonal face is nonremovable, but it could be *replaced* by a pentagon to give the distinct patch which appears in the catalogue as **I3:1**. Relationships similar to that between **I2:2** and **I3:1** can be found for larger generalized Stone–Wales patches, e.g. construction of **I3:4** and **I3:5** by replacement of one bridge hexagon of **I2:4**. With **I3:1**, again both fillings would usually be represented as distinct; with the addition of a spectator pentagon in the bay, for example, **I3:1** appears in Figure 5A of ref 15 and in Figure 5 of ref 17 and was identified by Chiu et al.<sup>19</sup> The long Stone–Wales transformations described by Balaban et al. are constructed by taking a string of  $2k-2$  peri-condensed hexagons with two pentagons on opposite sides at its ends, conserving the central zigzag path of  $2k$  vertices but switching in parallel all connections from the  $2k-2$  inner points to the periphery. Further generalization brings in even numbers of pentagons. All these and other variations are included in reduced form in the catalogue.

The third isomerization patch of the catalogue, **I2:3**, is the smallest of the star-like rearrangements found by Astakhova and Vinogradov<sup>16</sup> and discussed by Babic and Trinajstić.<sup>17</sup>

Whilst many of the isomerization patches are known, though here codified in a different way, the isomerization pairs offer many previously unrecognized types of transformation. As pointed out earlier, the pair transformations escape the classification of ref 16. The smallest pair **II:2:1** is already large, with a boundary of 26 vertices and illustrates the nonintuitive ways in which pentagons can be moved around on the surface of a fullerene once reconstruction of the interior of the patch is allowed.

Construction of the catalogue is an essentially mathematical process, yielding all possibilities consistent with the definitions. The strength of the approach is that when correctly implemented it will miss nothing out and that it is capable of uncovering nonobvious candidates. From the chemical point of view, the provision of the catalogue is only the beginning of the investigation. Many of the mathematically possible rearrangements imply large geometric change

and disruption of bonding that is likely to be costly in energy. On the other hand,<sup>18</sup> some processes that involve larger numbers of migrating bonds may be formally allowed under orbital symmetry rules, whereas apparently simpler transformations are forbidden. The role of adventitious extra atoms and small molecules in lowering activation barriers<sup>13</sup> complicates prediction of energetics. Existence of the catalogue offers the opportunity to make an unbiased survey of these and other possibilities.

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