Generalized Stone-Wales Transformations for Fullerene Graphs
Derived from Berge's Switching Theorem

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Abstract

Berge's switching theorem can be applied to fullerenes to connect all isomers within a set of fullerenes of vertex number n, $\{C_n\}$. Here we show that Berge's 2-switch operations are linked in a simple way to generalized Stone-Wales transformations (gSW). Some important examples with I_h-C_{240} and NS-T-C_{380} complete the investigation. The question remains if for fullerenes such gSW transformations are complete in the sense that from one chosen isomer the complete isomer set $\{C_n\}$ of a fixed vertex number n can be created.
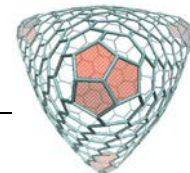
1. Introduction

A regular fullerene is a 3-regular cubic planar graph F that is generally describable as a mesh of (exactly) 12 variously fused pentagons, and surrounded by distorted graphenic fragments consisting in total of ($n/2-10$) hexagons as derived from Euler's polyhedral formula. Fullerenes excluding direct pentagon fusion are produced by the overlap of 12 nanocones and show a peculiar thermodynamic stability following the *isolated pentagon rule* (IPR) early observed by Kroto [1]. The number $N_{iso}(C_n)$ of regular fullerene isomers grows asymptotically as $N_{iso}(C_n) \sim O(n^9)$ with n being the number of carbon atoms (nodes or vertices) [2]. This polynomial growth also holds for sole IPR molecules: for example, C_{120} has 1,674,171 isomers of which 10,774 are IPR fullerenes. The generation of these fascinating hollow polyhedra poses therefore a challenge to mathematicians and chemists, which found some guidance in the publication of an atlas of fullerenes by Fowler, Manolopoulos almost two decades ago [3] containing the first database of fullerene structures up to C_{50} and IPR cages up to C_{100}. This important achievement worked as a stimulus for the creation of even more powerful and complete fullerene generators, like the *Buckygen* program [4,5], to construct and analyze all isomers up to C_{400} including fullerenes which do not contain any face spiral (NS), e.g. the two smallest ones being NS-*T*-NS-C_{380} and NS-D_3-C_{384}, followed most likely by NS-D_3-C_{440}.

One of the authors (see reference [6] and related links) and coworkers recently developed a general purpose and open-source computer package called *Fullerene*, which includes a comprehensive set of efficient algorithms to perform a graph theoretical, force-field, geometrical and topological analysis for any fullerene isomer, i.e. it produces 2D fullerene graphs (e.g. Schlegel diagrams) and accurate 3D fullerene structures in cartesian or internal coordinates. An accompanying fullerene database includes all general isomers up to C_{150} (for IPR isomers up to C_{200}), including the number of Hamiltonian cycles for general isomers up to C_{110} and for IPR isomers up to C_{122}. The main task of the program is to create the structure of a specific fullerene by applying all available computational techniques, like the Fowler-Manolopoulos ring-spiral algorithm, where the 12 ring spiral pentagon indices (RSPI) are used to uniquely build the molecular structure and to find fullerenes in the neighborhood of given ring-spiral pentagon indices [3]. The spiral algorithm has recently been generalized to allow for face-jumps allowing, for example, the construction of all NS-fullerenes [7]. The package also allows for Goldberg-Coxeter transformations of a fullerene [8], as well Endo-Kroto 2-vertex [9], Yoshida-Fowler 4- and 6-vertex [10] and Brinkmann-Fowler 6-vertex insertions [11,12].

Methods based on formal vertex insertions or deletions and formal isomerisations have proven to be very useful, as they allow the formal derivation of one fullerene graph from another. In particular, NS-fullerenes like *T*-C_{380} and D_3-C_{384}, that fail to be constructed using the face spiral
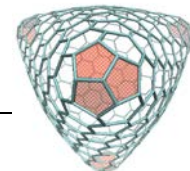
algorithm, can be derived from smaller fullerenes by proper sequences of vertices insertions [7]. In particular, the (standard) Stone-Wales transformation (SW transformation or pyracylene rotation) itself (see reference [13] and Figures 1-2) allows the *reversible* passage between fullerene isomers and, recursively used, it *partially* generates the isomeric space of a general C_n fullerene. For example, the buckminsterfullerene I_h-C_{60} cage is connected to the 94% of the whole C_{60} isomeric space by applying sequences of thirty SW flips or less [14]. More precisely, the early work [15] demonstrates how the 1812 C_{60} isomers are grouped in 13 independent sets, leaving 31 isolated isomers out of any SW pattern. The same research introduces a family of *generalized Stone-Wales transformations* (gSW$_L$) successfully applied to certain *linear* dispositions of fullerene faces to *completely* generate the isomeric spaces of both C_{60} and C_{70} fullerenes.

Figure 1. (a) For a general graph *G* the reversible 2-switch (2*s*) rearranges the edges in such a way that two pairs of unconnected atoms "receive" the *pair of edges* initially shared with other nearby atoms; (b) on a fullerene graph *F*, 2*s* reproduces the standard SW bond rotation by interchanging the positions of 2 pentagons and 2 hexagons; (c) the same SW rotation corresponds to the rotation of a *single* edge in the dual fullerene representation, dual(*F*). Red and blue circles represent pentagons and hexagons respectively.
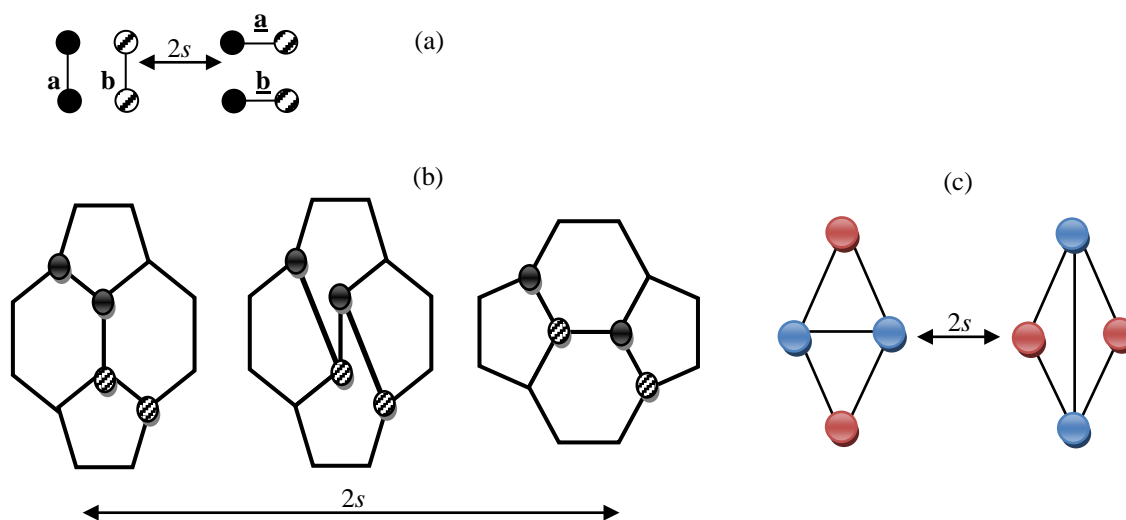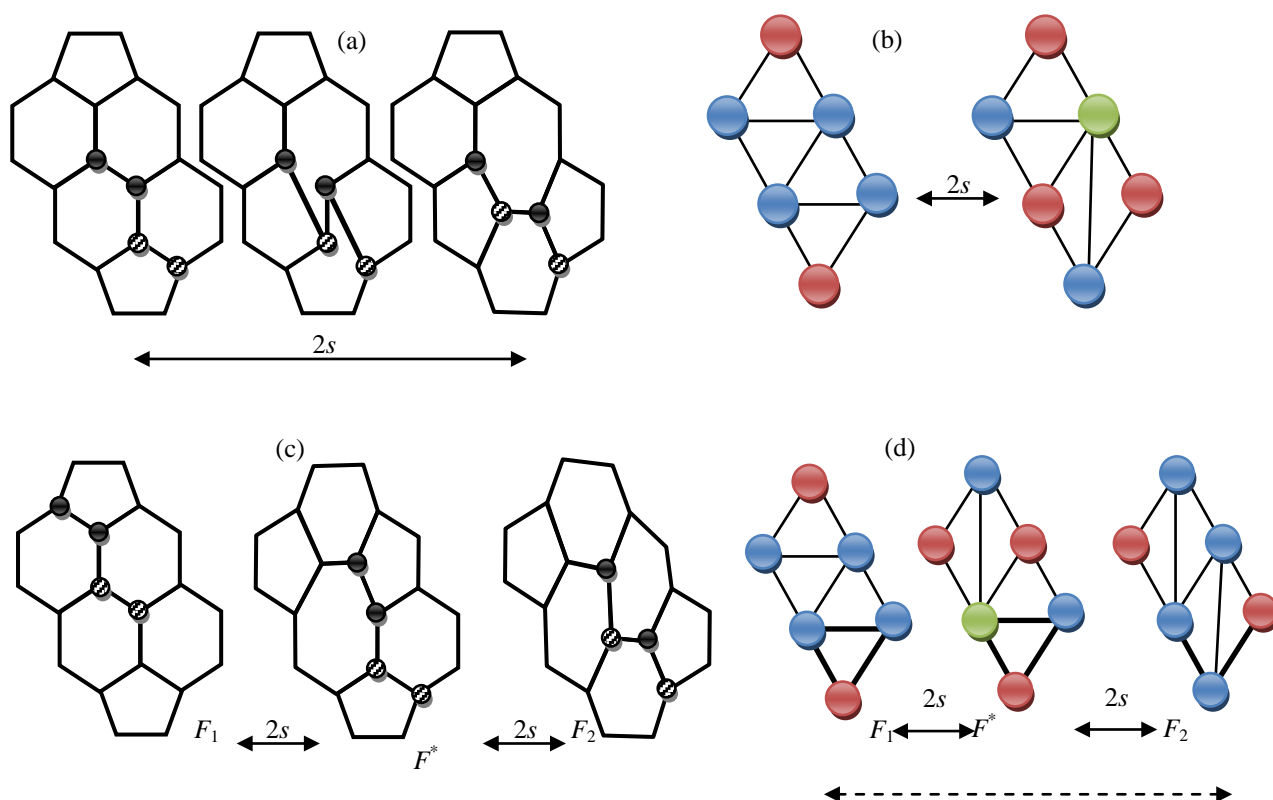

For the generation of fullerenes it would be useful to start with one specific isomer C_n (which can easily be constructed even for the largest fullerenes), and to have an efficient algorithm at hand to subsequently create a complete set of isomers within a specific vertex number, i.e. $C_n \rightarrow \{C_n\}$. This would complement the patch replacement algorithm of Brinkmann and co-workers [4]. Formally, such a method is given by Berge's switching theorem [16], which connects two graphs (under certain conditions as outlined below) by a sequence of 2-switch operations shown in Figure 1a. However, it
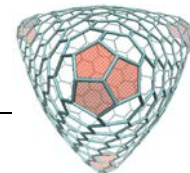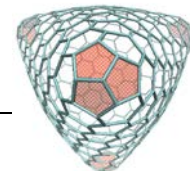
remains to be seen if an efficient algorithm of low polynomial order using this theorem can be found for the generation of all isomers within a set $\{C_n\}$ of fullerenes.

Figure 2. (a) The represented 2-switch starts from a fullerene fragment (left) but fails in producing a regular fullerene resulting in an extra pentagon and one heptagon. (b) This invalid rearrangement is obtained in the dual graph by rotating one bond. (c) A sequence made of two 2-switches, which reversibly connects two valid fullerenic regions F_1 and F_2 and its dual representation (d). Red, blue and green circles represent pentagons, hexagons and heptagons respectively.

As a first step in this direction, we analyze the mechanism for the generation and transformation of fullerene isomers by considering Berge's switching theorem and its implications over the interconnections of cubic graphs preserving the number of nodes n and the number of bonds (edges). In the next section a simple introduction to Berge's theorem will be provided and the relation with some classes of generalized Stone-Wales transformations evidenced with some original examples including the nonspiral T-C_{380} fullerene. Then, from the application of Berge's theorem on fullerene isomerisation it may be conjectured that *any given pair of isomers of a C_n fullerene is reversibly connected by a sequence of generalized SW transformation*.

Present theoretical findings enable new algorithmic approaches to describe and generate fullerenic structures. This note provides an original look into fullerene skeletons and suggests a new family of topological transforms able to connect all pairs of isomers of any given C_n fullerenic cage.

2. Berge's switching theorem

On a given simple graph $G(V,E)$, where V is the vertex and E the edge set, a 2-switch operation ($2s$) replaces two graph edges **a** and **b** with new edges **<u>a</u>** and **<u>b</u>** between nodes initially unconnected, see Figure 1a. In a cubic graph of a fullerene $F(V,E)$ each vertex v_i ($i = 1, \ldots, n$) has the same degree (e.g. the same number of bonds), i.e. $d_F(v_i)=3 \ \forall v_i \in V$. The four nodes involved in the 2-switch considered here are in close neighborhood. Figure 1 presents a *valid* 2-switch applied to a fullerene fragment, which obeys the extra constraint of producing a *valid* fullerene portion by conserving the number of pentagons and the number of total hexagons in the fullerene graph, i.e. $F_1 \rightarrow F_2$ where F_1 and F_2 are both fullerene graphs consisting of pentagons and hexagons only. This combination of topological requirements reproduces the well-known Stone-Wales rotation.

The illustrations in Figure 1 show the general bonds rearrangements caused by a $2s$ operation in a generic graph G, and, more important, they evidence that the ordinary SW rotation on a fullerene may be described as a legitimate 2-switch involving *two molecular* bonds. Note that the SW transformation simply corresponds to the rotation of a *single edge* (diagonal flip) in the dual representation of a fullerene (Figure 1c), dual(F), a graph made of ($n/2+2$) vertices (twelve nodes are of degree 5 and the remaining ones of degree 6). For the triangulation of surfaces, such diagonal flips have been investigated by Negami [17].

Further insights into $2s$ movements and their relationship with SW rearrangements on portion of fullerenes are provided in Figure 2. The top part illustrates a 2-switch ending however with a *non-regular fullerene portion* exhibiting an extra pentagon and a heptagon. Figure 2c and 2d show instead a *valid sequence* of two consecutive 2-switches converting the fullerene portion F_1 made of 2 pentagons and 4 hexagons in the new fullerenic fragments F_2 which is isomeric to the initial one but with a *different disposition* of the internal edges. The two fragments F_1 and F_2 have therefore different topologies and, in general, may have different geometrical symmetries, i.e. result in non-isomorphic graphs; this fact naturally reverberates on the overall molecular structure of the two involved C_n isomers: *generally the action of the 2-switch sequence results in non-isomorphic graphs for the two interconnected C_n fullerenes*.

As already noted, the resulting intermediate graph F^* obtained from the first 2-switch operation shown in Figure 2 *does not correspond to the portion of a regular fullerene*. This fact adds some difficulties in the search of valid 2-switch sequences, able to interconvert regular fullerene isomers, but also *opens up the way for producing non-regular fullerenes containing faces other than pentagons and hexagons*. An effective tool generating those transformations needs in fact to consider not only the local properties of the molecular graph but also its long-range topology features, aiming for peculiar
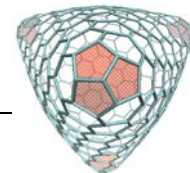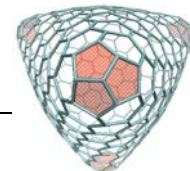
subgraphs having a structure *globally* suitable for these kind of operations. A valid sequence of local 2-switches as used here may be seen, from a purely algorithmic point of view, as a *non-local instantaneous transformations of suitable portions (or subgraphs) of the fullerene surface*, a very intriguing novel way of describing fullerene isomerisation mechanisms. The first example of such a mechanism is given in Figure 2d, where the two subgraphs F_1 and F_2 may be connected by a *non-local instantaneous transformation* which corresponds to the generalized Stone-Wales *linear* transformation gSW^L with size $\eta=1$ introduced in [15], which also includes the standard SW rotation with size $\eta=0$. Details about gSW^L and a new family of generalized Stone-Wales rearrangements will be introduced in the next section with some selected applications. For the moment, it is important having established the relationship between *valid 2-switches sequences and generalized Stone-Wales transformations* for fullerenes.

Figure 1 and 2 also evidence how in the dual graph the generation of 2-switches largely simplifies, enabling the (future) search for efficient algorithms generating valid sequences of 2-switches in *dual* C_n fullerenes graph and, more generally, in any graphenic systems with various types of carbon rings, like heptagons, octagons and so on. Similar graphical methods have been recently introduced to generate graphenic defective structures obtained by isomeric series of SW rotations [18].

After having presented the connection between 2-switch and generalized SW transformations, the main graph-theoretical result related to the 2-switch mechanism is represented by the following *switching theorem* due to Berge (1973) [16]:

- *Two graphs G and H having a common vertex set V satisfying $d_G(v_i)=d_H(v_i) \; \forall \; v_i \in V$ if and only if H can be obtained from G by a sequence of 2-switches.* (1)

The shorthand for this kind of relationships between graphs is *G=2s(H)*. Berge's switching theorem was proven by Havel [19] (see also [20]). Applications of this theorem for networks are already known [21]. Clearly, this graph property implies an important consequence on the topological structure of graphs *G* and *H* in case they represent two isomers of a given fullerene C_n. Both molecules share in fact the same number *n* of 3-conencted vertices being $d_G(v_i)=d_H(v_i)=3$ for all carbon atoms v_i, and, as a consequence of Berge's theorem, *these two molecules are connected by a sequence of 2-switches*. Considering that *G* and *H* are valid C_n fullerenes, it descends from the previous graphic examples that the search for that special sequence also becomes the search for specific gSWs:

- *Given two fullerene isomers G and H one has to find the specific sequence of generalized SW transformations, which in force of Berge's theorem exists and transforms G in H and vice-versa.* (2)

The necessity of including gSW derives also from the proven impossibility (mentioned in the introductory section) of connecting any pairs of C_{60} fullerenes by using standard SW transformations [8,9]. The list of available gSW one may invoke to connect two fullerene isomers is so far limited to the class of linear generalized SW transformations $gSW^L(\eta)$ [15] and to the newly discovered family, the *radial* generalized SW transformations $gSW^R(\eta)$ that will be introduced in the next section. On the basis of Berge's theorem (1) and the present conjecture (2) (yet to be proven) one may expect that the group A of generalized SW transformations is sufficiently large to connect, for any molecular size n, any pairs of C_n isomers by a proper sequence of elements of A. By considering gSW transformations as special kind of 2-switch operations, the reversible sequence of 2-switches interconnecting C_n fullerenes F_1 and F_2 is therefore summarized as a sequence of k elements a_i of A:

$$F_1 = 2s(F_2) = A(F_2) = a_{1*}a_{2*}...._{*}a_k \; F_2 \qquad (3)$$

Operators a_i may act on different portions of the graph representing the fullerene F_1. It is easy to check that the sequence of k gSW transformations in (3) is not uniquely defined by considering the topological structure of the two interconnected isomeric graphs F_1 and F_2 and may be achieved in different ways, by varying the total number k and the types of the single a_i transforms. The exhaustive search of the members of the group A is therefore an important computational subject of future studies. We mention however, that trivially 2-switches are more general than gSW transformations. While gSW transformations maintain planarity of the graph, 2-switches in general do not.

3. Generalized Stone-Wales transformations

The mechanism underlying the linear generalized SW transformations $gSW^L(\eta)$ is graphically explicated in Figure 3a which generalizes the previous one shown in Figure 2c. It basically mirrors the external pentagon-hexagon pairs 5|6 by rearranging the internal η pairs of hexagons. This mechanism is made very clear in the dual graph representation, Figure 3b. Pivotal faces – the two pairs 5|6 – are colored in red (pentagons) and blue (hexagons, the remaining ones are in gray. The intermediate 2η faces actually may also be pentagons since all gSW do not vary the connectivity along the boundary of
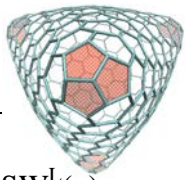
the considered fullerene portion. In spite of this quite basic graph-transform, sequences of $gSW^L(\eta)$ operations with $\eta=0,1,2,3$ span the whole isomeric space of C_{60} made of 1,812 distinct isomers (3,532 when enantiomeric pairs are considered as two distinct cages); when $gSW^L(4)$ rearrangements are taken into consideration, even C_{70} isomeric space is totally generable starting from *any* C_{70} fullerene just by applying proper sequences of $gSW^L(\eta)$ operations with $\eta=0,1,2,3,4$ (see more details in the original work [9]). These quite interesting results clearly derive from Berge's theorem (1) on 2-switches, and authorize the search of other classes of gSW, being the infinite linear transformations $gSW^L(\eta)$ and their various combinations the first example of elements of the group *A* producing the isomerisations of a given C_n fullerene.

Figure 3. Graphical representation of the linear generalized SW transformations $gSW^L(\eta)$ in the direct (a) and the dual (b) space. The $\eta=1,2$ sequences of 2-switches shown respect the external topological connectivity of the region, and reversibly connect two valid C_n fullerene isomers. For linear gSW the parameter η equals the number of pairs of internal faces and may assumes any integer values for arbitrarily large *n*. Red, blue and gray elements represent pivotal pentagons, hexagons and internal faces respectively.
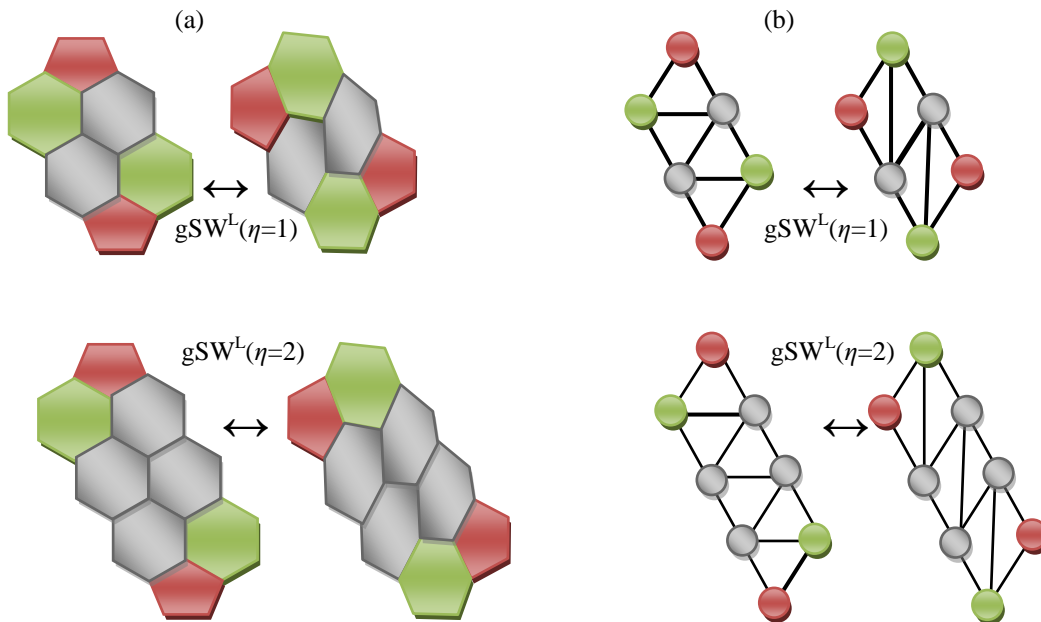

The quest for new *A* elements results here in a first elegant solution by considering the *radial* (instead of *linear*) disposition of pairs of hexagon and pentagons that, after the gSW rearrangement, mutually exchange their positions. Figures 4a and 4b show the *radial* generalized SW transformations $gSW^R(\eta)$, which rotates the fullerene region like in the standard SW rotation of Figures 1b and 1c. Pivotal faces are again two pentagons and two
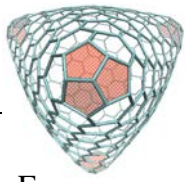
hexagons colored in red (pentagons) and blue (hexagons), the remaining rings are in gray. For the radial case, the size η of $gSW^R(\eta)$ counts the number of internal hexagons bridging the two pivotal hexagons.

Figure 4. Graphical representation of the radial generalized SW transformations $gSW^R(\eta)$ in the direct (a) and the dual (b) space. The $\eta=1,2$ reversible sequences of 2-switches shown respect the boundary topology connecting two valid C_n fullerene isomers. Red, blue and gray elements represent pivotal pentagons, hexagons and internal faces respectively. For the radial gSW, the parameter η equals the number of 6-rings bridging pivotal hexagons and may assume any integer values for arbitrarily large n.
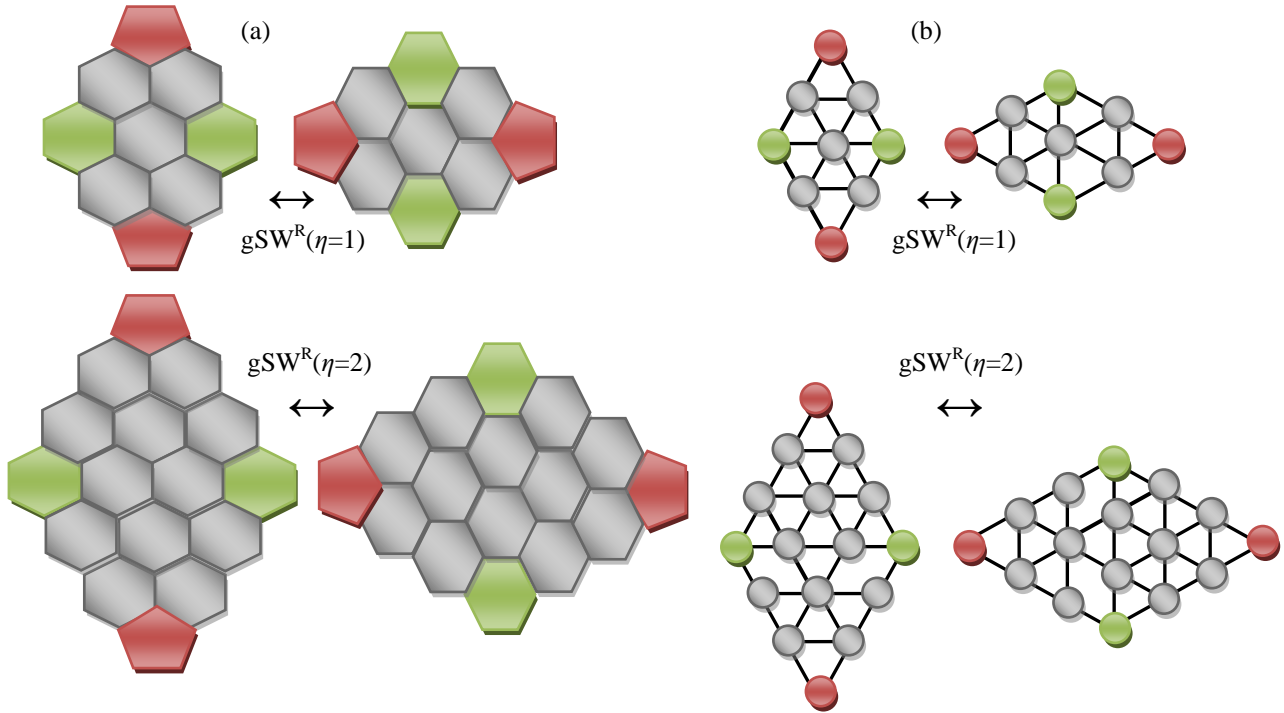
At $\eta=0$, this class of transformations $gSW^R(\eta)$ reduces to the standard SW flip according to the operator equality:

$$gSW^L(\eta) = gSW^R(\eta) = SW \quad \text{for } \eta=0 \tag{4}$$

As an element of A, the SW is indicated by a_0. SW is a *single* 2-switch transform, whereas for $\eta>0$ all gSW consist of a *sequence* of 2-switches. The role of SW as a common element in eq. (4) arises from the starting pivotal faces (a pair of pentagons and a pair of hexagons) these three kinds of transforms SW, $gSW^L(\eta)$, $gSW^R(\eta)$ have in common, and this property may change for gSW arising from an alternative topological mechanism. This aspect will be the subject of future computational investigations.
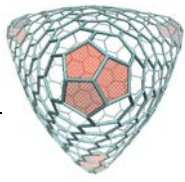
## 4. Notable cases of a $F_2 = A(F_1)$ fullerene transformation

The first application of the isomerisation methods developed here concerns a truly distinguished fullerene, the non-spiral (NS) T-C_{380} cage [22,23]. Looking like a hexagon-tessellated regular pyramid with a group of 3 fused pentagons at each apex, it is the smallest fullerene escaping the Fowler-Manolopoulos face-spiral encoding algorithm [3]. Its generation requires – as already mentioned – more sophisticated tools like a general face spiral algorithm including jumps [7] as listed in Table 1 for NS-T-C_{380}. Its topological skeleton however admits along the pyramidal edges 6 linear generalized Stone-Wales transformations of size $\eta=8$ (equivalent to the 6 edges of a tetrahedron). Figure 5a shows the pristine NS-T-C_{380} isomer and one of the pivotal pairs of the $gSW^L(7)$ (in orange the pentagon and green the hexagon). The results of this $gSW^L(7)$ transformation is a new C_2-C_{380} isomer which exhibits a number of face spirals, Table 2. Due to its symmetry, this fullerene has 120 distinct face spirals. From Berge's theorem (1) or our gSW conjecture (2) present it trivially follows that the NS-fullerene T-C_{380} can be constructed from spiral fullerene like C_2-C_{380} by subsequent $2s$ rearrangements constituting the proper $\underline{a}=gSW^L(7)$ overall transform:

$$\text{NS-}T\text{-}C_{380} = A(C_2\text{-}C_{380}) = \underline{a}(C_2\text{-}C_{380}) \tag{5}$$

Figure 5. C_{380} isomers interconnected by linear gSW transformations: NS-T-C_{380} (a); the spiral fullerene $gSW^L(7)(T\text{-}C_{380}) = C_2$-$C_{380}$ (b); the $a_0[gSW^L(7)(T\text{-}C_{380})] = C_1$-$C_{380}$ (c). Structures are force-field optimized using program Fullerene [6].
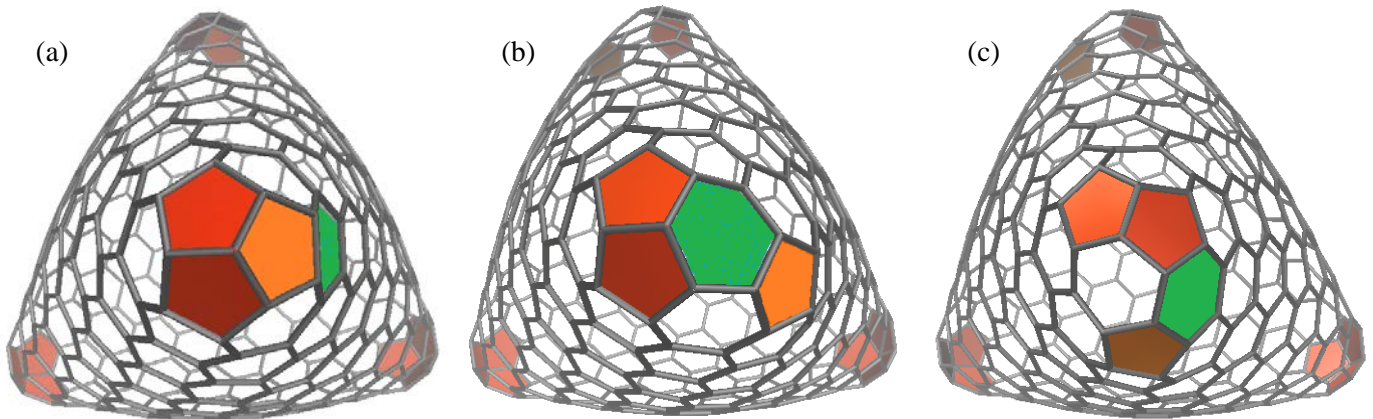
Being gSW reversible, it is not necessary to use distinct symbols to differentiate between the NS-T-$C_{380} \rightarrow C_2$-C_{380} transformation and the C_2-$C_{380} \rightarrow$ NS-T-C_{380} back-transform. C_2-C_{380} appearing in relation (5) as a spiral fullerene *seed* to generate NS-fullerene T-C_{380} is just the representative of a large class of fullerenes one may easily find by applying gSW sequences (3). Conjecture (2) states
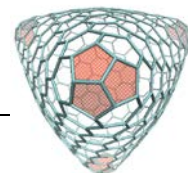
something more, it indicates that that for any C_{380} isomer at least one element $p \in A$ exists in such a way that NS-T-$C_{380} = p(C_{380})$.

Table 1. Canonical face spiral pentagon indices (FSPI) and jumps (for NS-T-C_{380} only) for various fullerenes studied obtained from program Fullerene [6]. For the definition of the general spiral algorithm used see [7].

Fullerene	FSPI												jumps
I_h-C_{240}	1	33	37	41	45	49	75	79	83	87	91	122	0
gSW^R(3) (I_h-C_{240})	1	8	36	42	48	71	77	81	85	105	109	113	0
T-C_{380}	45	70	71	82	83	110	119	120	144	184	185	192	110, 3
gSW^L(7) (T-C_{380})	2	8	9	98	123	132	133	151	160	168	169	186	0
SW[gSW^L(7) (T-C_{380})]	2	8	20	110	112	129	130	139	157	170	171	187	0

Table 2. Topological parameters for various fullerenes studied obtained from program Fullerene [6]. Point group symmetry (PG), number of spirals (N_s), number of symmetry distinct spirals (N_{ds}), Fowler-Manolopoulos neighboring pentagon index (N_P) and strain parameter (σ_H), band gap (ε_{HL}) in eV, Wiener index (W), Szeged index (Sz), Estrada index (Es), Balaban index (B), topological efficiency index (ρ), exact volume (V) and volume of convex hull (V_{CH}) in Å^3, exact surface area (A) and surface area of convex hull (A_{CH}) in Å^2, isoperimetric quotient (q_{IP}), and minimum distance sphere deformation parameter (D_{MDS}) in %. For definitions see [6].

| Property	I_h-C_{240}	gSW^R(3)(I_h-C_{240})	T-C_{380}	gSW^L(7) (T-C_{380})	SW[gSW^L(7) (T-C_{380})]
PGS	I_h	C_{2v}	T	C_2	C_1
N_s	1080	1076	0	320	319
N_{ds}	9	269	0	160	319
N_P	0	0	12	8	8
σ_H	0.4979	0.5332	0.5416	0.6020	0.6020
ε_{HL}	1.499	0.583	0.434	0.061	0.080
W	277440	277264	864762	865872	865880
Sz	4250880	4298248	17592456	17595803	17596604
Es	786.30	786.30	1244.29	1244.29	1244.29
B	0.459470	0.459826	0.372707	0.372115	0.372112
ρ	1.0	1.030568	1.054292	1.060805	1.060815
V	1438.5	1292.6	2280.4	2306.5	2306.8
V_{CH}	1449.8	1324.7	2412.0	2430.3	2430.2
A	626.5	598.6	947.6	948.3	948.3
A_{CH}	627.3	604.8	979.5	977.4	976.2
q_{IP}	0.9516	0.8810	0.6913	0.7055	0.7057
D_{MDS}	1.874	5.816	17.43	17.09	16.86
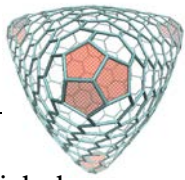
By applying a simple Stone-Wales transformation a_0 to C_2-C_{380} at the part which has undergone a gSW^L(7), one obtains the C_1-C_{380} = a_0 (C_2-C_{380}) isomer as shown in Figure 5c. Applying SW two both transformed patterns on opposite ends of the tetrahedron one simple gets the original fullerene back, a_0'$_*a_0$ (C_2-C_{380}) = C_2-C_{380}.

As a further application of the radial rearrangement gSW^R(η) we take the highly symmetric I_h-C_{240} fullerene. For each pentagon on the surface, its topological structure contains 5 gSW^R(3) patterns, one of these is shown in Figure 6a where green (red) faces indicate pivotal hexagons (pentagons). The result of the 2s sequence represented by the $\underline{b}$=gSW^R(3) reversible transform, yields the C_{2v}-C_{240} isomer of lower symmetry represented in Figure 6b:
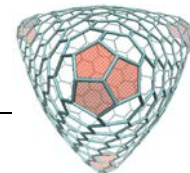
$$I_h\text{-}C_{240} = A(C_{2v}\text{-}C_{240}) = \underline{b}(C_{2v}\text{-}C_{240}) \qquad (6)$$

Figure 6. C_{240} isomers interconnected by radial gSW transformations: I_h-C_{240} (a); gSW^R(3)(I_h-C_{240}) = C_{2v}-C_{240} (b). Structures are force-field optimized using program Fullerene [6].
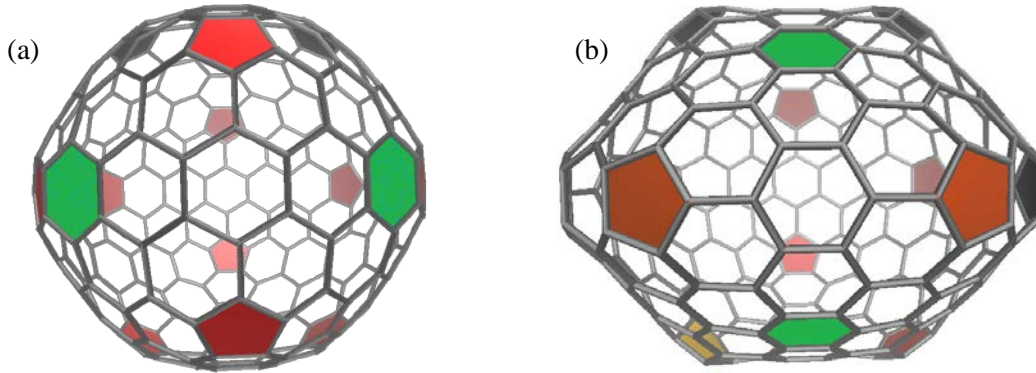
The C_{2v}-C_{240} cage contains many other gSW patterns and, more generally, also for this fullerene conjecture (2) requires that operation (7) is valid for *any pairs* of C_{240} fullerenes when a proper gSW sequence p is selected: (C_{240})' = $p(C_{240})$. For general C_n fullerenes, conjecture (2) arising from Berge's theorem poses interesting computational and applicative questions, that will be addressed in future studies.

Our present study is completed by listing of canonical face spiral pentagon indices (FSPI) (Table 1) and topological parameters for the fullerenes including the required jump for NS-T-C_{380} (Table 2). We mention some interesting topological features of I_h-C_{240} leading to its peculiar topological efficiency ρ=1 [6,24-26]. Compared to I_h-C_{60}, which has 60 symmetry-equivalent atoms each with 9 coordination shells with population 3,6,8,10,10,10,8,3,1, this icosahedral C_{240} cage has instead 3 symmetry-distinct sets of atoms each with 19 coordination shells: 60 atoms with population 3, 6, 8, 11, 13, 16, 18, 20, 20, 20, 20, 20, 18, 15, 13, 8, 6, 3, 1; 60 atoms with population

3,6,9,11,14,16,18,18,20, 20 20,18,18,16,11,11,6,3,1 and the remaining 120 nodes with population 3, 6 9, 12, 14,16,17,19,19,20,19,19,17,15,14,9,7,3,1. Topologically, the molecule has therefore a (2:1:1) C^{13} NMR resonance theoretical spectrum. The relative contribution to the Wiener index $W=277,440$ for I_h-C_{240} is however common $w=2,312$, and this leads to a minimal molecular topological efficiency (maximizing its sphericality) with $\rho=2W/nw=1$. I_h-C_{240} is therefore the smallest fullerene molecule with maximal sphericality even with non-symmetry equivalent atoms.

5. Conclusion

Our studies show that generalized Stone-Wales transformations belong to the class of 2-switches. The application of Berge's theorem points towards a possible conjecture, which implies the coverage of the whole isomeric space of any C_n fullerene by using only proper gSW sequences leading to fullerene graphs which remain planar and cubic. Moreover, the original Fowler-Manolopoulos ring-spiral algorithm [3] scales like $O(n^{12})$, while the isomer space covered by the pentagons is very sparse scaling like $O(n^9)$ [2]. The gSW algorithm, if complete, would only cover fullerenes with valid pentagon indices. Future theoretical and computer investigations are necessary to investigate this rather intriguing feature.

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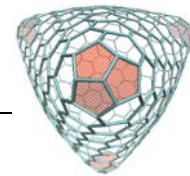
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