Разбиения поверхностей на многоугольники и задачи, пришедшие из физики, химии и биологии

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Лекция 3

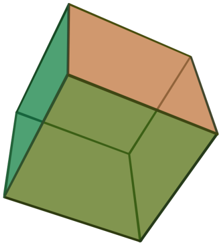
Зигзаги на простых разбиениях

Пусть M^2 – поверхность с фиксированным простым разбиением.
Путём Петри называется рёберный путь, такой что никакие три последовательных ребра не лежат в одной грани.
Зигзагом называется замкнутый путь Петри.
Простым называется зигзаг без самопересечений.

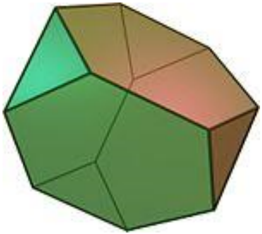
Следствие

Простой зигзаг разбивает поверхность фуллерена на два простых разбиения диска, каждое из которых содержит ровно 6 пятиугольников.

Простой многогранник называется флаговым, если любой набор его попарно пересекающихся гиперграней $F_{i_1}, \dots, F_{i_k}$: $\forall a, b \quad F_{i_a} \cap F_b \neq \varnothing$, имеет непустое пересечение $F_{i_1} \cap \dots \cap F_{i_k} \neq \varnothing$.

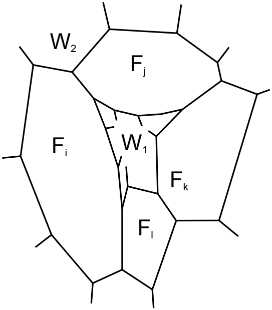


Флаговый многогранник



Нефлаговый многогранник

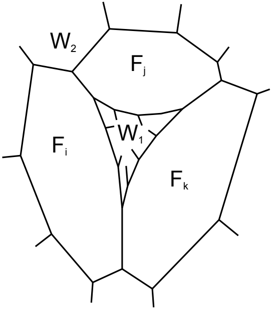
Let P be a simple convex 3-polytope. A ***k-belt*** *is a cyclic sequence $(F_1, \dots, F_k)$ of 2-faces, such that $F_{i_1} \cap \dots \cap F_{i_r} \neq \varnothing$ if and only if $\{i_1, \dots, i_r\} \in \{\{1,2\}, \dots, \{k-1, k\}, \{k, 1\}\}$.*



4-belt of a simple 3-polytope.

Non-flag 3-polytopes

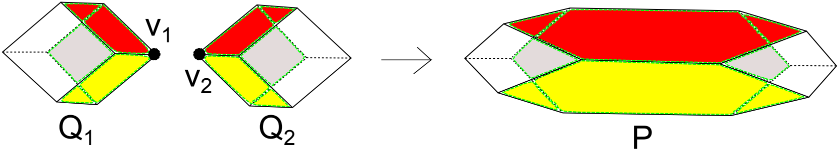
Simple 3-polytope P is not flag *if and only if either $P = \Delta^3$, or P contains a* 3-belt.



If we remove the 3-belt from the surface of a polytope, we obtain two parts W_1 and W_2, homeomorphic to disks.

Non-flag 3-polytopes as connected sums

The existence of a 3-belt is equivalent to the fact that P is combinatorially equivalent to a connected sum $P = Q_1 \#_{v_1, v_2} Q_2$ of two simple 3-polytopes Q_1 and Q_2 along vertices v_1 and v_2.



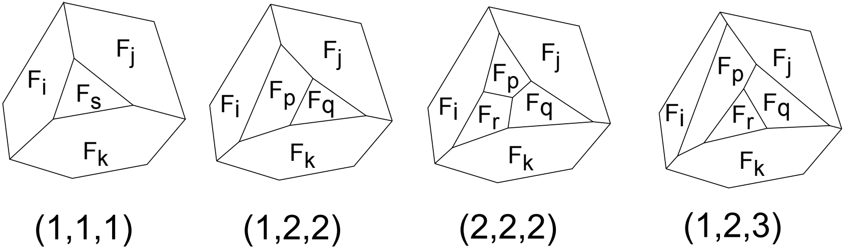
The part W_i appears if we remove from the surface of the polytope Q_i the facets containing the vertex v_i, $i = 1, 2$.

Fullerenes as flag polytopes

Теорема (E,15)

Any fullerene has no 3-belts, that is it is a flag polytope.

The proof is based on the following result about fullerenes.
Let the 3-belt (F_i, F_j, F_k) divide the surface of a fullerene P into two parts W_1 and W_2, and W_1 does not contain 3-belts. Then P contains one of the following fragments



This is impossible since each fragment has a triangle or a quadrangle.

4-belts and 5-belts of fullerenes

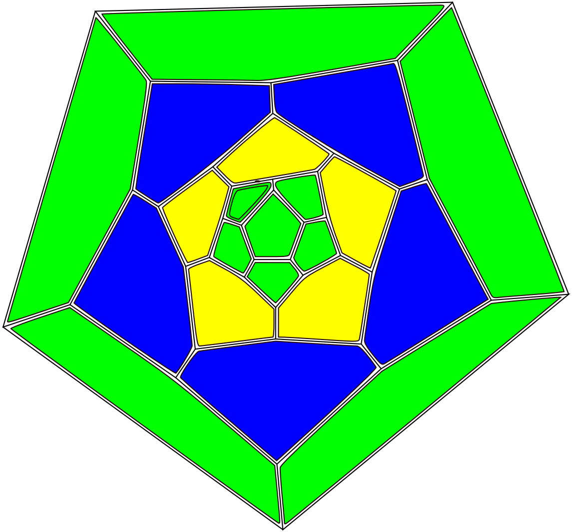
Теорема

Any fullerene has no 4-belts.

Теорема

Any fullerene P has $12 + k$ belts, where 12 belts surround 12 pentagonal faces and $k \geqslant 0$. If $k > 0$, then P consists of two «dodecahedral caps» and k hexagonal 5-belts between them, where any hexagon in a belt is incident with neighboring hexagons by opposite edges.

Fullerene with 2 hexagonal 5-belts

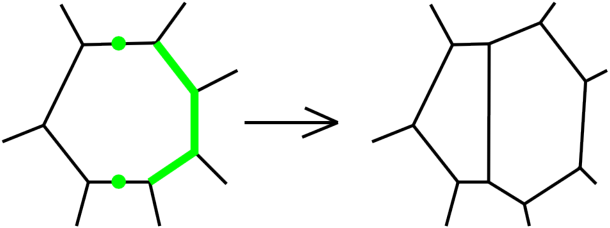


(s, k)-truncations

Let F_i be a k-gonal face of a simple 3-polytope P.

- *choose s subsequent edges of F_i;*
- *rotate the supporting hyperplane of F_i around the axis passing through the midpoints of adjacent two edges (one on each side);*
- *take the corresponding hyperplane truncation.*

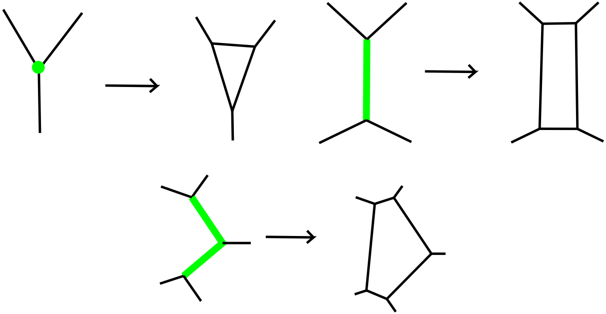
We call it (s, k)-truncation.



$(3, 7)$-truncation

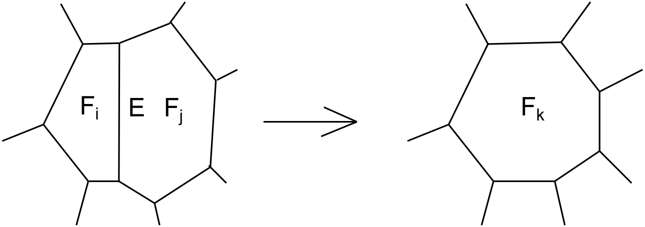
Теорема (Eberhard, Brückner, XIX)

Any simple 3-polytope is combinatorially equivalent to a polytope that is obtained from the tetrahedron by a sequence of vertex, edge and $(2, k)$-truncations.



Straightening along the edge

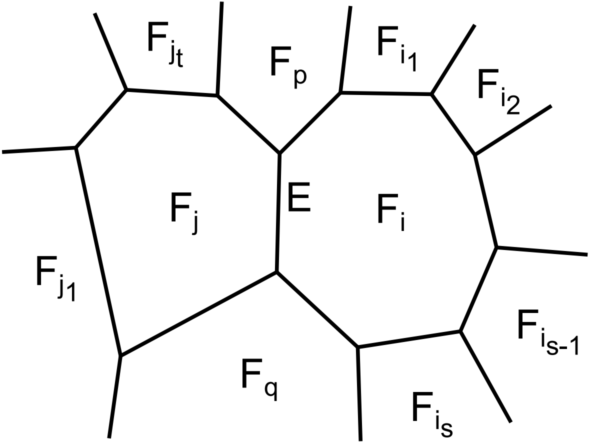
Let $E = F_i \cap F_j$ be an edge such that p-gon F_i and q-gon F_j do not belong together to any 3-belt. Then there is a combinatorial operation of straightening along E.



The result is a combinatorial polytope with a $(p+q-4)$-gonal face F_k obtained from F_i and F_j.

The straightening is an inverse operation to $(p-3, p+q-4)$- or $(q-3, p+q-4)$-truncations along edges of F_k.

Possibility of strengthening



It is possible to apply the straightening along the edge $E = F_i \cap F_j$ *if and only if* $\{F_{i_1}, \ldots, F_{i_s}\} \cap \{F_{j_1}, \ldots, F_{j_t}\} = \varnothing$.

Construction of flag 3-polytopes

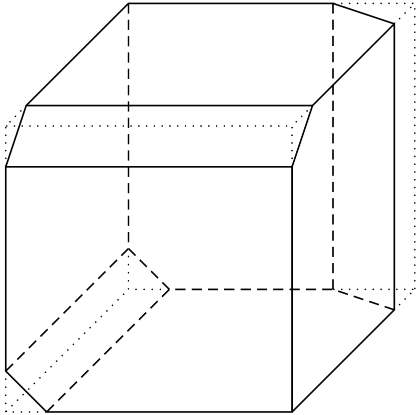
Proposition (V. Volodin, 2011)

A simple 3-polytope P is flag if and only if it admits the straightening along any edge E of P.

Теорема (E, 15)

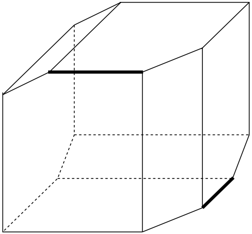
A simple 3-polytope is flag if and only if it is combinatorially equivalent to a polytope obtained from the cube by a sequence of edge truncations and $(2, k)$-truncations, $k \geqslant 6$.

Realization of the Stasheff polytope

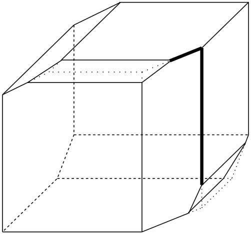


A realization of the Stasheff polytope using edge-truncations (V. Buchstaber, 2007)

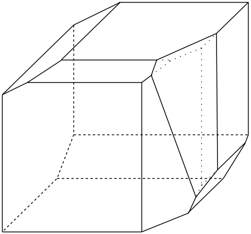
Realization of the dodecahedron



$(p_4, p_5, p_6) = (3, 6, 0)$



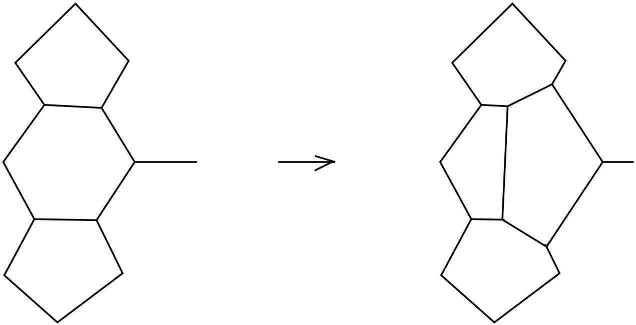
$(p_4, p_5, p_6) = (2, 8, 1)$



$(p_4, p_5, p_6) = (0, 12, 0)$

- first apply 3 edge-truncations to the cube to obtain the associahedron;
- then apply 2 edge-truncations of bold edges;
- at last apply $(2, 6)$-truncation of two bold edges.

Перестройка Эндо-Крото



- Перестройка Эндо-Крото увеличивает p_6 на 1.
- При помощи последовательности перестроек Эндо-Крото из бочки можно получить фуллерен с любым $p_6 = k$, $k \geqslant 2$.

Characterization of the Endo-Kroto operation

- The Endo-Kroto operation is a $(2, 6)$-truncation.
- The only (s, k)-truncation that gives a fullerene from a fullerene is an Endo-Kroto operation.

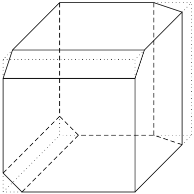
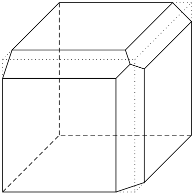
For a simple 3-polytope P let

$$P = \{\boldsymbol{x} \in \mathbb{R}^n \colon \boldsymbol{a}_i\boldsymbol{x} + b_i \geqslant 0, i = 1, \dots, m\}$$

be an irredundant representation and $G(P)$ be the 1-skeleton of P. Then for a subgraph $\Gamma \subset G(P)$ without isolated vertices define a graph-truncation

$$P_{\Gamma,\varepsilon} = P \cap \{\boldsymbol{x} \in \mathbb{R}^n \colon (\boldsymbol{a}_i + \boldsymbol{a}_j)\boldsymbol{x} + (b_i + b_j) \geqslant \varepsilon, F_i \cap F_j \in \Gamma\}$$

The combinatorial type does not depend on ε, if $\varepsilon > 0$ is small enough. Denote it by P_Γ.

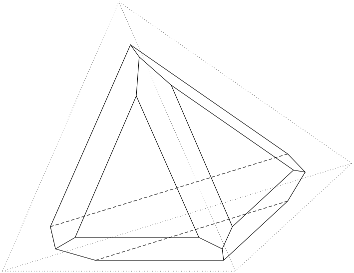
 

Different realizations of the associahedron.

Cutting off all edges

The polytope $P_{G(P)}$ is obtained from P by cutting off of all the edges.

$$p_k(P_{G(P)}) = \begin{cases} p_k(P), & k \neq 6 \\ p_k(P) + f_1(P), & k = 6 \end{cases}$$



$$(p_3, p_4, p_5, p_6) = (4, 0, 0, 6)$$

Cutting off of all the edges of a simplex.

The graph $\Gamma \subset G(P)$ is admissible if any it's vertex has valency 1 or 3.

Теорема

For a simple 3-polytope P the polytope P_Γ is simple if and only Γ is admissible

Теорема

For a simple 3-polytope P and an admissible graph $\Gamma \subset G(P)$ the polytope P_Γ is flag if and only if for any 3-belt (F_i, F_j, F_k) in P one of the edges $F_i \cap F_j$, $F_j \cap F_k$ and $F_k \cap F_i$ belongs to Γ, and for any triangular face F_i the induced subgraph $\Gamma \cap F_i$ has isolates vertices.

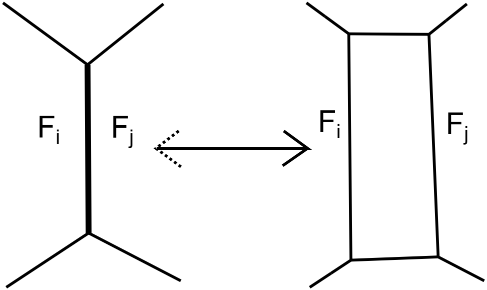
Graph-truncation and (s, k)-truncation

An edge-truncation (that is a $(1, k)$-truncation) is the only operation that is simultaneously a graph-truncation and an (s, k)-truncation.

- *A graph-truncation is a monotonic operation. That is, let P be a simple polytope and $\Gamma \subset P$ be an admissible graph. Then $p_k(P_\Gamma) \geqslant p_k(P)$ for all k and there exists l such that $p_l(P_\Gamma) > p_l(P)$.*
- *(s, k)-truncation is not a monotonic operation. For example, let Q be a polytope such that the dodecahedron P is obtained from Q by a $(2, 6)$-truncation. Then*

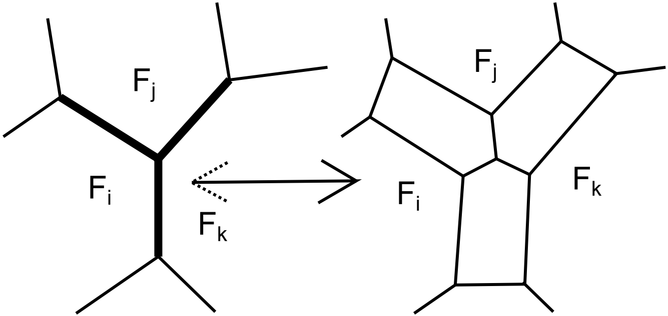
$$p_4(Q) = 2 \geqslant 0 = p_4(P), \quad p_5(Q) = 8 \leqslant 12 = p_5(P),$$
$$p_6(Q) = 1 \geqslant 0 = p_6(P).$$

First nontrivial graph-truncations



The inverse operation
is applicable if and only if
$F_i \cap F_j = \varnothing$.

First nontrivial graph-truncations



The inverse operation
is applicable if and only if
$F_i \cap F_j = F_i \cap F_k = F_j \cap F_k = \varnothing$.

Теорема (E,14)

For every sequence $(p_k | 4 \leqslant k \neq 6)$ *of nonnegative integers satisfying*

$$2p_4 + p_5 = 12 + \sum_{k \geqslant 7} (k-6)p_k,$$

there exists an integer p_6 *and a flag simple 3-polytope* P^3 *with* $p_k = p_k(P^3)$ *for all* $k \geqslant 4$.

If P has no triangles then the polytope $P_{G(P)}$ is flag.

Construction of *IPR*-fullerenes

- An Endo-Kroto operation can not give an *IPR*-fullerene.
- For a fullerene P the polytope $P_{G(P)}$ is an *IPR*-fullerene with $p_6(P_{G(P)}) = p_6(P) + f_1(P)$.
- For the dodecahedron the corresponding *IPR*-fullerene C_{80} has 80 vertices and is highly symmetric.

Fullerenes obtained by a graph-truncation

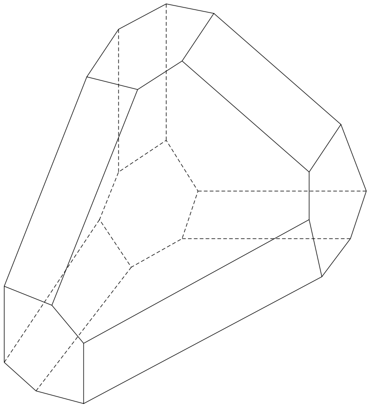
The edge $E \in \Gamma$ is a shout of the 2-face F for the graph $\Gamma \subset G(P)$, if $E \cap F$ is a 1-valent vertex of Γ.

Теорема

Let P be a simple 3-polytope and $\Gamma \subset P$ be an admissible graph. Then P_Γ is a fullerene if and only if

- *Γ does not have isolated edges;*
- *$p_k(P) = 0$ for $k \geqslant 7$;*
- *any triangular face of P has two or three shouts;*
- *any quadrangular face of P has one or two shouts;*
- *any pentagonal face of P has at most one shout;*
- *any hexagonal face of P has no shouts.*

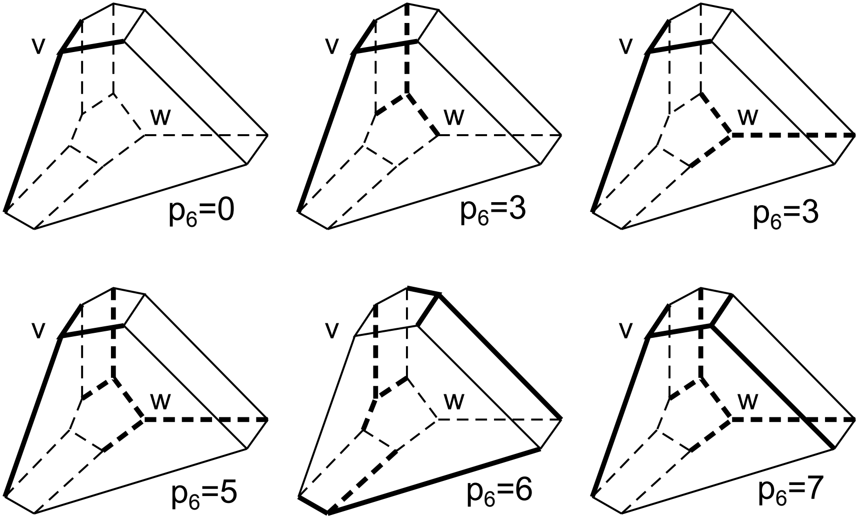
Graph-truncations of the permutohedron



Proposition

We can not obtain a fullerene as a graph-truncation of the permutohedron.

All graphs up to the symmetry on the associahedron that give fullerenes



Let P be a fullerene and $\Gamma \subset P$ be an admissible graph.

Следствие

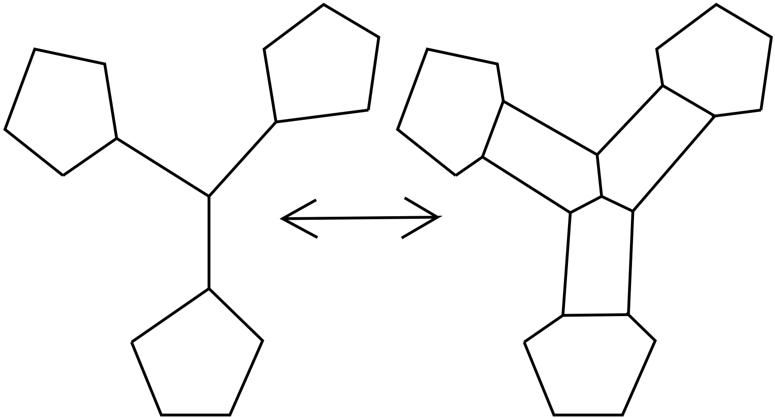
P_Γ is a fullerene if and only if

- *Γ does not have isolated edges;*
- *any hanging edge of Γ is a shout of a pentagon;*
- *different hanging edges correspond to different pentagons;*

If P_Γ is not a fullerene, then we can not obtain a fullerene from it by any sequence of graph-truncations.

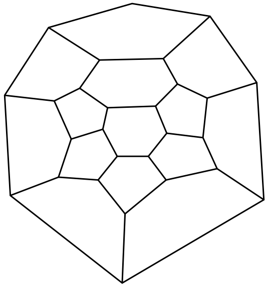
Graph-truncations of fullerenes

The first nontrivial graph-truncation gives the following operation on fullerenes, which is always defined in both directions.



Simple edge cycles on fullerenes

- A simple cycle in $G(P)$ divides a boundary of a fullerene P into two disks W_1 and W_2 with induced simple partitions.
- There is a bijection between the boundary vertices of W_1 and W_2 that maps the vertex of valency i to the vertex of valency $5-i$.
- For each disk W_1 and W_2 we have $\mu_2 \neq 1$ and $\mu_3 \neq 1$.



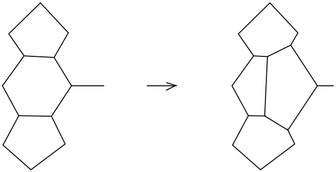
A simple partition of a disk which can not appear as W_1 or W_2.

Surgery of fullerenes

By a surgery of a fullerene we mean the operation of replacement of W_1 by a simple partition W_1' of D^2 into 5- and 6-gons such that there exists a bijection between the boundary vertices $v_1', \dots, v_p'$ of W_1' and $v_1, \dots, v_p$ of W_1 ordered cyclically that

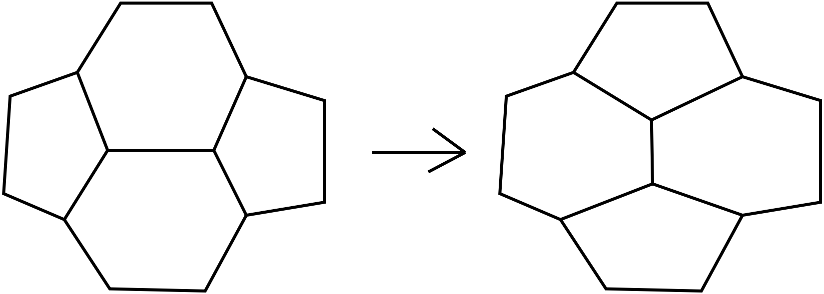
- *preserves the valences of vertices;*
- *has the form $v_i' \to v_{(s+i) \bmod p}$ or $v_i' \to v_{(s-i) \bmod p}$ for some s.*

The result is again a fullerene.



An Endo-Kroto operation gives a surgery of fullerenes.

Stone-Wales operation



- A Stone-Wales operation can produce an isomer;
- It is a flip;
- It is an example of a surgery.

Кольцо Стенли-Райснера простого многогранника

Пусть $\{F_1, \dots, F_m\}$ — множество гиперграней простого многогранника P. Кольцо Стэнли–Райснера над $\mathbb{Z}$ определяется как

$$\mathbb{Z}[P] = \mathbb{Z}[v_1, \dots, v_m]/(v_{i_1} \dots v_{i_k} = 0, \ \textit{if } F_{i_1} \cap \dots \cap F_{i_k} = \varnothing).$$

- Кольцо Стэнли–Райснера флагового многогранника задается квадратичными соотношениями: соотношения имеют вид $v_i v_j = 0$: $F_i \cap F_j = \varnothing$.
- Два многогранника комбинаторно эквивалентны тогда и только тогда, когда их кольца Стэнли–Райснера изоморфны.

Каждый фуллерен является простым флаговым многогранником

Квадратичная алгебра Стенли-Райснера является кошулевой.

Квадратично двойственной алгеброй фуллерена *называется квадратично двойственная алгебра его кольца Стенли-Райснера.*

Структура квадратично-двойственно алгебры фуллерена полностью описывается матрицей инциденций графа граней фуллерена, которая в физике и химии называется его «топологической матрицей».

На основе этой матрицы в квантовой химии проводится расчёт физико-химических свойств фуллерена.

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