

Discrete Geometry, Combinatorics and Applications

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Research Overview

Our main topics are interdisciplinary: Distance Design and Structures in Nature. At spring 2009 Springer will publish "Encyclopedia of Distances" (about 600 pages) by Michel and Elena Deza. These distances are particularly crucial, for example, in Computational Biology, Image Analysis, Speech Recognition, and Information Retrieval.

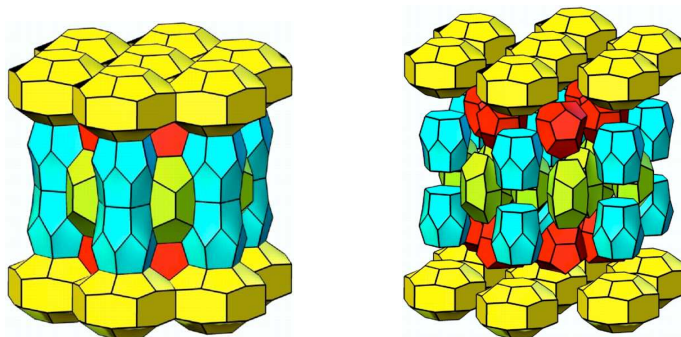
Main structures considered are chemical graphs such as (1-skeletons of) fullerenes and n -polycycles. A *fullerene* F_n is an n -vertex polyhedron with only hexagonal and 12 pentagonal faces. Fullerenes or their duals are ubiquitous in nanoworld (Organic Chemistry and Virology).

Three recent results

I. Space fullerenes and metallic alloys.

A *space fullerene* is a 4-valent 3-periodic \mathbb{E}^3 -tiling by fullerenes. *Frank-Kasper structure* is such tiling by fullerenes with isolated hexagons: $F_{20}(I_h)$, $F_{24}(D_{6d})$, $F_{26}(D_{3h})$, $F_{28}(T_d)$. 24 of them are known, all as structures of *metallic alloys*, *clathrate hydrates*, *zeolites* or *soap froths*.

Deza and Shtogrin found unique known non-Frank-Kasper space fullerene:

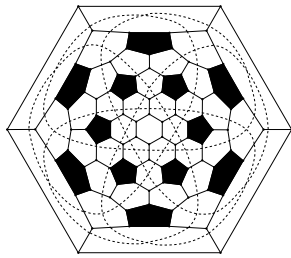


Dutour, Deza and Delgado, 2008, enumerated Frank-Kasper structures with at most 16 fullerenes in the reduced unit cell. 8 among 30 found belong to the list of 24 known ones: compounds called A_{15} , C_{15} , Z , C_{14} , δ , $p\delta$, σ and K_7Cs_6 . 3 of 22 new ones disprove the old conjecture by Yarmolyuk-Kripyakevich, 1974, on the proportion of 20-, 24-, 26-, 28-vertex fullerenes in the unit cell. So, a new challenge to Material Science is to check the existence of metallic alloys, zeolites, etc., having one of 22 new geometrical structures

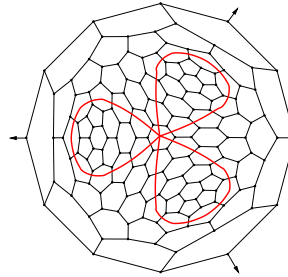
II. Railroads in fullerenes (Deza, Dutour and Fowler).

A *railroad* in a fullerene is a circuit of hexagons which are adjacent to two their neighbors on opposite faces. Discovery of these knots and links inside of plane fullerene graph opened new vistas on combinatorics of fullerenes.

Fullerene is called *IPR* if its pentagons are isolated.



$F_{96}(D_{6d})$, first IPR fullerene
with self-intersecting
railroad

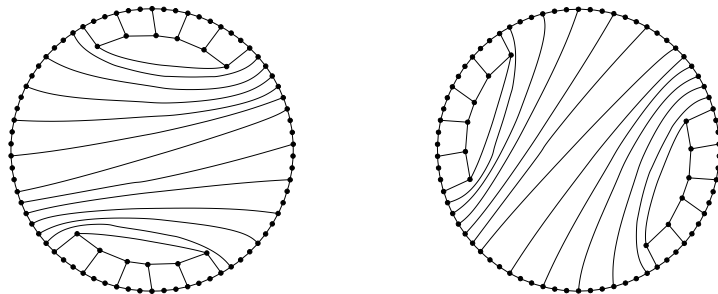


$F_{176}(C_{3v})$, first fullerene
with triply intersecting
railroad

III. Ambiguous polycycle boundaries (Deza and Shtogrin).

An *n-polycycle* is a 2-connected plane graph such that all interior faces are n -gons, interior vertices are of degree 3 and boundary vertices are of degree 2 or 3. Recent discovery, that two large enough n -polycycles can have the same boundary, had an impact on enumeration of n -polycycles.

The smallest *ambiguous* (i.e. admitting 2 fillings by n -polycycles) boundary for the main applicable case, $n = 6$, is given below.



International Activities: Michel Deza serves as Editor-in-chief of European Journal of Combinatorics and editor for 9 international journals.

Awards: Michel Deza is Founding Fellow of Institute of Combinatorics and Vice-President of European Academy of Sciences.

Publications

- M.Deza and M.Dutour, *Geometry of Chemical Graphs*, Cambridge Univ. Press, 2008.
- M.Deza and E.Deza, *Encyclopedia of Distances*, Springer, to appear.
- M.Deza, M.Dutour and M.Shtogrin, *Elementary elliptic (R, q) -polycycles*, a chapter in *Analytical, Computational and Statistical Approaches for Network Analysis*, ed. by M.Dehmer and F.Emmert-Streib, to appear.
- M.Deza and V.Grishukhin, *More about the 52 four-dimensional paralleleptopes*, Taiwanese J. Math. **12-4**, pp. 901–916, 2008.
- M.Deza, M.Dutour and S.Shpectorov, *Hypercube embedding of Wythoffians*, Ars Math. Contemp. **1**, pp. 99–111, 2008.
- M.Deza and M.Shtogrin, *New examples of generalized fullerenes*, Russian Math. Surveys, **64-1**, to appear.
- M.Deza and S.Shpectorov, *Polyhexes that are l_1 graphs*, European J. Combinatorics, to appear.