STUDIA UBB CHEMIA, LIX, 3, 2014 (p. 103 - 108)
(RECOMMENDED CITATION)

# TOPOLOGICAL SYMMETRY OF MULTI-SHELL ICOSAHEDRAL CLUSTERS

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**ABSTRACT.** Topological symmetry is referred to the maximum possible symmetry achievable by a given molecular structure; it can be performed either by permutations on the adjacency matrix or by calculating the values of some topological indices. The equivalence classes of vertices/atoms of the multi-shell nanostructures under study were solved by using a topological index computed on the layer matrix of atom surrounding rings and compared with the results of matrix permutation. A centrality order of vertices in multi-shell clusters is given. The design of nanostructures was performed by map operations as implemented in our original CVNET and Nano Studio software programs.

***Keywords:*** *Multi-shell cage, centrality index, vertex equivalence class, automorphism.*

## INTRODUCTION

Molecular structures show various types of geometrical symmetry [1-4]. Geometrical symmetry is reflected in several molecular properties, which are dependent on the spatial structure of molecules. Molecular topology reveals a *topological symmetry* (*i.e.*, constitutional symmetry), defined in terms of *connectivity* and expresses equivalence relationships among elements of graph: vertices, bonds, faces or larger subgraphs.

Using the notions of the Group action [3], in which every element of the group acts like as a one–to–one mapping, the group $G$ is said to act on a set $X$ when there is a function $\varphi$ such that $\phi : G \times X \longrightarrow X$ and for any element $x \in X$,

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there exists: $\phi(g, \varphi(h,x)) = \phi(gh,x)$, for all $g,h \in G$, with $\phi(e,x) = x$, $e$ being the identity element of $G$. The mapping $\phi$ is called a group action while the set $\{\phi(gx) \mid g \in G\}$ is called the *orbit* of $x$. For a permutation $\sigma$ on $n$ objects, the permutation matrix is an $n \times n$ matrix $P_\sigma$, with elements $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. For any permutation $\sigma$ and $\tau$ on $n$ objects, $P_\sigma P_\tau = P_{\sigma\tau}$, while the set of all permutation matrices is a group isomorphic to the symmetry group $S_n$ on $n$ symbols. A permutation $\sigma$ of the vertices of a graph $H(V,E)$ ($V$ being the set of vertices and $E$ the set of edges in $H$) belongs to an automorphism group $G$ if one satisfies $P_\sigma^t A P_\sigma = A$, where $A$ is the adjacency matrix of the graph $H$. Given $Aut(H) = \{\sigma_1, \ldots, \sigma_m\}$, the matrix $S_G = [s_{ij}]$, where $s_{ij} = \sigma_i(j)$ is called a solution matrix for $H$ and its calculation will provide the automorphism group of $H$.

Given a graph $H(V,E)$ and the automorphism group $Aut(H)$, two vertices, $i, j \in V$ are called *equivalent* if $\{\phi(ij) \mid i,j \in Aut(H)\}$, in other words, they belong to the same orbit of automorphisms.

Suppose $v_1, v_2, \ldots, v_m$ are $m$ disjoint *automorphic partitions* of the set of vertices $V(H)$, then: $V = V_{v1} \cup V_{v2} \cup \ldots \cup V_{vm}$ and $V_{v_i} \cap V_{v_j} = \varnothing$.

Let now consider a vertex invariant, $In = In_1, In_2, \ldots, In_m$, which assigns a value $In_i$ to the vertex $i$. Two vertices $i$ and $j$ of a molecular graph (with vertices meaning the atoms and edges the bonds in the molecule) belong to the same *invariant class IC* if $In_i = In_j$. The partitioning in *classes* of vertices/atoms leads to $m$ classes, with $v_1, v_2, \ldots v_m$ atoms in each class; such a partitioning may differ from the *orbits of automorphism* i.e. *classes of equivalence*, since no vertex invariant is known so far to always discriminate two non-equivalent vertices in any graph. The classes of vertices are eventually *ordered* according to some rules.

A given binary relation ~ on a set $A$ is said to be an *equivalence relation* if and only if it is: reflexive($x \sim x$); symmetric ($x \sim y \Rightarrow y \sim x$) and transitive ($x \sim y \, and \, y \sim z \Rightarrow x \sim z$).

It is worthy to mention that topological symmetry equals the maximum geometrical symmetry a molecular graph can have.

A layer matrix [5] is built up on a layer partition of a vertex $i$ in the graph $G(V,E)$:

$$G(i) = \{G(i)_j, j \in [0, ecc_i] \quad and \quad v \in G(i)_j \Leftrightarrow d_{iv} = j\}$$

where $ecc_i$ is the eccentricity of $i$ (*i.e.*, the largest distance from $i$ to the other vertices of $G$). The entries in a layer matrix, **LM**, collect the vertex property $p_v$ (a topological, chemical, or physical property) for all the vertices $v$ belonging to the layer $G(i)_j$:

$$[\mathbf{LM}]_{ij} = \sum_{v \in G(i)_j} p_v \, ,$$

for vertices located at distance $j$ from vertex $i$. The matrix **LM** is defined as

$$\mathbf{LM}\,(G) = \{\,[\mathbf{LM}]_{ij};\; i \in V(G);\; j \in [0, d(G)]\,\}$$

where $d(G)$ is the diameter of the graph. The dimensions of the matrix is $N\times(d(G)+1)$; the zero-distance column is just the column of vertex properties.The most simple and essential layer matrix is the *counting* property (*i.e*., the existence of a vertex in a given position / at a given distance is counted by 1, and zero, otherwise). In the following, as a property, the count of rings *R* around each vertex is considered, the layer matrix being **LR**.

Layer matrices are used to derive the indices of *centrality C*(**LM**), that quantify the centrality of vertices and finally the inside centrality of a graph

$$C(\mathbf{LM})_i = \left[\sum_{k=1}^{ecc_i}\left([\mathbf{LM}]_{ik}^{2k}\right)^{1/(ecc_i)^2}\right]^{-1}$$

where $ecc_i$ is the eccentricity of *i.*

## RESULTS AND DISCUSSION

### Design of multi-shell cages

The cages under study represent 3D-tessellations, recently developed by Diudea [1], achieved by map operations [6-8], as implemented by the original software CVNET [9].

In building the cluster $C_{750}$, the sequence of operations is as follows: TRS($P_4(C_{60})$)_330; $S_2(C_{60})$_420; TRS($P_4(C_{60})$)@$S_2(C_{60})$_750 (Figure 1).

The structure TRS($P_4(C_{60})$)@$S_2(C_{60})$_750 = $C_{60}((C_{20})_{60})$_750 is a "spongy" one, with the central hollow of exact topology of TRS($P_4(C_{60})$)_330. It is a $C_{20}$-tessellation: formally, every point in the graph of $C_{60}(I_h)$ is changed by a cage $C_{20}$; notation $C_{60}((C_{20})_{60})$ means $60\times(C_{20})$ within the topology of $C_{60}(I_h)$. The joining of the two halves was made by our original software Nano Studio [10].

Cluster $C_{408}$ was made by all-point truncation of the Diudea's cluster Tr(Diu45)_408, where $Diu_{45}$=(IcoP@$IcoP_{12}$)_45. It is the intersection of 12×Tr(IcoP)_84 (related to Samson's cluster_104), the core being the $13^{ne}$Tr(IcoP)_84 (Figure 2).

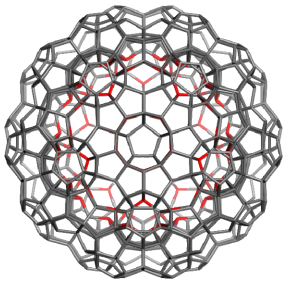
### Topological symmetry

Topological symmetry is referred to the maximum possible symmetry achievable by a given molecular structure; it can be performed either by permutations on the adjacency matrix [1-3] or by calculating the value of some topological indices [1-4]. In the following tables, the equivalence classes of vertices/atoms are presented in their descending centrality, calculated on the layer matrix of surrounding rings RL. The atom type, eg. 3^3.5^2.6^4 reads: $R_3\times3$; $R_5\times2$; $R_6\times4$, $R_3$ being a triangle, $R_5$ a pentagon and $R_6$ a hexagon.

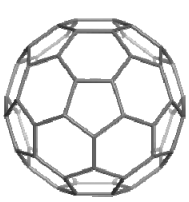
The symmetry for the icosahedral structures in Figures 1 and 2 was computed by the GAP software program as being

$$C_2 \times A_5 = I_h;\ |I_h| = 120.$$

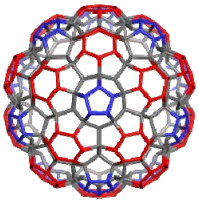
It confirmed the equivalence classed established by the centrality index (Tables 1 and 2).



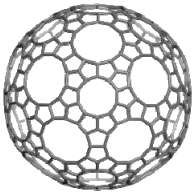
**$C_{60}((C_{20})_{60})\_750$**
TRS($P_4(C_{60})$)@($S_2(C_{60})$420)_750



$C_{60}$



TRS($P_4(C_{60})$)_330

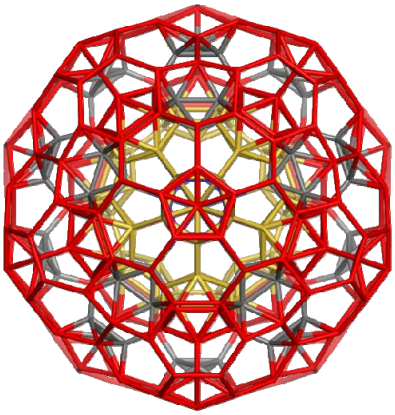


$S_2(C_{60})$_420

**Figure 1.** $C_{750}$ and its substructures

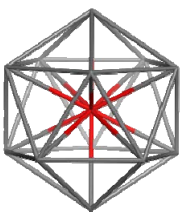
**Table 1.** $C_{750}$: Automorphism group = $C_2 \times A_5 = I_h;|I_h| = 120$ (cf. GAP permutations). Equivalence classes of atoms in the descending order of their centrality cf. LR matrix.

| Class | Centrality signature | No. Elements | Vertex degree | Atom type |
|---|---|---|---|---|
| 1 | 0.0425537487829127 | 60 | 4 | 5^5 |
| 2 | 0.0425405656366799 | 30 | 4 | 5^5 |
| 3 | 0.0408741428983785 | 60 | 3 | 5^3 |
| 4 | 0.0403249632533878 | 60 | 4 | 5^6 |
| 5 | 0.0403215210989583 | 60 | 4 | 5^5.6 |
| 6 | 0.0403184110690464 | 60 | 4 | 5^5.6 |
| 7 | 0.0380980964599947 | 60 | 4 | 5^5 |
| 8 | 0.0380776127196794 | 60 | 4 | 5^5 |
| 9 | 0.0380525586272046 | 60 | 4 | 5^5 |
| 10 | 0.0363966020960237 | 60 | 3 | 5^3 |
| 11 | 0.0363899446618803 | 60 | 3 | 5^3 |
| 12 | 0.0363398403991418 | 120 | 3 | 5^3 |

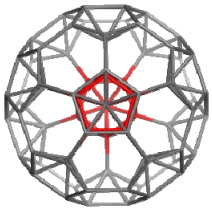


**Tr(IcoP)84@((Tr(IcoP)84)$_{12}$_408**

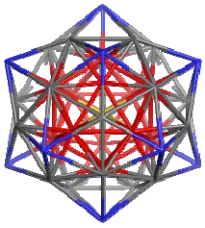
(Ico@($TT_{20}$)@($Ico_{12}$;$TT_{20}$;$TT_{30}$)@($Py_5$;$TT_5$)$_{12}$_408
Tr(Diu45)_408



IcoP_13



Tr(IcoP)_84



Diu_45=IcoP@IcoP12_45

**Figure 2.** $C_{408}$ and its substructures

**Table 2.** $C_{408}$: Automorphism group = $C_2 \times A_5 = I_h$; $|I_h| = 120$ (cf. GAP permutations). Equivalence classes of atoms in the descending order of their centrality cf. LR matrix.

| Class | Centrality signature | No. Elements | Vertex degree | Atom type |
|---|---|---|---|---|
| 1 | 0.0825432266953615 | 12 | 6 | 3^5.5^5.6^5 |
| 2 | 0.0723127280340924 | 12 | 6 | 3^5.5^5.6^5 |
| 3 | 0.064639289864084 | 60 | 6 | 3^5.5^5.6^5 |
| 4 | 0.0580357622307322 | 60 | 6 | 3^5.5^5.6^5 |
| 5 | 0.0572358681133143 | 12 | 6 | 3^5.5^5.6^5 |
| 6 | 0.0564467194639707 | 60 | 6 | 3^5.5^2.6^5 |
| 7 | 0.0552836553218085 | 60 | 5 | 3^3.5^2.6^4 |
| 8 | 0.0512081941907237 | 12 | 6 | 3^5.6^5 |
| 9 | 0.0505895569851173 | 60 | 4 | 3^2.5.6^3 |
| 10 | 0.0467456474901417 | 60 | 4 | 3^2.5.6^3 |

## COMPUTATIONAL DETAILS

The multi-shell cages $C_{750}$ and $C_{408}$, Figure 1, were built up on computer by using CVNET [9] software program and their topology analysed. The vertices were partitioned in classes function of the surrounding rings and then by their centrality index. The calculations were made by Nano-Studio [10]. The automorphism data for both these structures were calculated by the GAP (Groups, Algorithms and Programming) program.

## CONCLUSION

Classes of equivalence of vertices/atoms of the multi-shell icosahedral nanostructures were solved by using the Centrality topological index, computed on the layer matrix of all rings around atoms and confirmed by the results of matrix permutation. Future work will analyze the equivalence classes of edges/ bonds and faces/rings by transforming the actual cages in their medial and dual graphs, respectively.

## ACKNOWLEDGMENTS

The work was supported by the Romanian CNCSIS-UEFISCSU project, PN-II IDEI 129/2010, PN-II-ID-PCE-2011-3-0346.

## REFERENCES

[1]. M. Diudea, in *Diamond and Related Nanostructures*, eds. M.V. Diudea and C.L. Nagy, Diamond and Related Nanostructures, Springer, Dordrecht, **2013**, Chap.19, p. 335.
[2]. A.R. Ashrafi, F. Kooperazan-Moftakhar, M.V. Diudea, M. Stefu, in: M.V. Diudea, C.L. Nagy, Eds., Diamond and Related Nanostructures,Springer, Dordrecht, **2013**, Chap. 18, p. 321.
[3]. Hungerford, Thomas W. *Algebra*. Reprint of the 1974 original. Graduate Texts in Mathematics, 73. Springer–Verlag, New York–Berlin, **1980**.
[4]. M.V. Diudea and C.L. Nagy, Periodic Nanostructures, Springer, Dordrecht, **2007**.
[5]. M.V. Diudea and O. Ursu, Layer matrices and distance property descriptors, *Indian J. Chem. A*, **2003**, *42*, 1283.
[6]. M.V. Diudea, M. Stefu, P.E. John and A. Graovac, Generalized operations on maps, *Croat. Chem. Acta,* **2006**, *79*, 355.
[7]. M.V. Diudea, Nanoporous Carbon Allotropes by Septupling Map Operations, *J. Chem. Inf. Model.*, **2005***, 45*, 1002.
[8]. M.V. Diudea, Capra-a leapfrog related operation on maps, *Studia UBB Chemia*, **2003**, *48* (2), 3.
[9]. M. Stefu and M.V. Diudea, CageVersatile_CVNET, Babes-Bolyai Univ. Cluj, **2005**.
[10]. Cs.L. Nagy, M.V. Diudea, NANO-Studio, Babes-Bolyai Univ. Cluj, **2009**.