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Topological Symmetry of C_{60}-Related Multi-Shell Clusters

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Abstract. Multi-shell clusters can be constructed, on the ground of C_{60} topology, by using operations on maps. Cell duals for some of the studied structures were also designed and next transformed into even more complex clusters. Topology of such clusters was analysed by the aid of a centrality index, computed on layer matrices of vertex properties. Vertices were partitioned into classes of equivalence and ordered according to their centrality. Finally, the vertex classification according to topological description was confirmed by the automorphisms counted by permuting the elements in the corresponding adjacency matrices.

1 Introduction

Symmetry (from Greek συμμετρία symmetria "agreement in dimensions, due proportion, arrangement") commonly refers to harmony of proportions in realization of a composition [1]. The simplest symmetry is the mirror symmetry. In Mathematics, symmetry refers to some operations acting on geometric or other regularities of a mathematical object that leave the object invariant.

Molecular geometric symmetry is involved in several properties, such as dipole moments, IR vibrations, ^{13}C-NMR signals etc., strongly dependent on the spatial structure of molecules. Molecular topology reveals a different type of symmetry: *topological symmetry* or constitutional symmetry, with *connectivity* being the building principle of molecules. Topological symmetry expresses equivalence relationships among elements of graph: vertices, bonds, faces or larger subgraphs, in a formalism taken from Set and Group Theories. The geometrical aspects are disregarded [2,3].

In the theory of Group action [4,5], a group G is said to act on a set X if there is a function ϕ such that $\phi : G \times X \longrightarrow X$ and for any element $x \in X$, there exists: $\phi(g, \phi(h,x)) = \phi(gh,x)$, for all $g,h \in G$, with $\phi(e,x) = x$, e being the identity element of G. The mapping ϕ is called a group action while the set $\{\phi(gx) \mid g \in \mathrm{G}\}$ is called the *orbit* of x. For a permutation σ on n objects, there is a permutation matrix P_{σ}, of dimensions $n \times n$, of which elements are $x_{ij} = 1$ if there is a permutation $i=\sigma(j)$ and 0 otherwise. For any permutation σ and τ 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 σ 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 the relation $P_{\sigma}^{t}AP_{\sigma} = A$, where A is the adjacency matrix of the graph H. Given $Aut(H) = \{\sigma_1, \ldots, \sigma_m\}$, the matrix $S_G = [s_{ij}]$, with $s_{ij} = \sigma_i(j)$ is called a solution matrix for H; calculation of these solutions will provide the automorphism group of H.

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

The *automorphic partitions* of the vertex set $V(H)$: v_1, v_2,..., v_m are disjoint, that is $V = V_{v1} \cup V_{v2} \cup \ldots \cup V_{vm}$ and $V_{v_i} \cap V_{v_j} = \varnothing$. If the partitioning is provided by a topological vertex invariant: $In = In_1, In_2, \ldots, In_m$, the invariant orbits/classes may differ from the orbits of automorphism, since no vertex invariant is known so far to always discriminate two non-equivalent vertices in any graph [3]. To detail the above, two vertices i and j of a molecular graph (with vertices meaning the atoms and edges the bonds in the molecule) are equivalent (i.e., belong to the same *invariant class IC*) if $In_i = In_j$. Recall that a binary relation ~ on a set A is an *equivalence relation* if and only if it is: reflexive ($x \sim x$); symmetric ($x \sim y \Rightarrow y \sim x$) and transitive ($x \sim y \text{ and } y \sim z \Rightarrow x \sim z$).These equivalence classes are eventually *ordered* according to some rules.

A layer matrix [3,6-8] is built on a layer partition of a vertex *i* in the graph *H*(*V*,*E*), defined as

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

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

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

The matrix **LM** is a collection of the above entries, for all vertices and layers, up to the graph diameter *d*(*H*):

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

LM is a non-square matrix, of dimensions $N\times(d(G)+1)$; the zero-distance column is just the column of vertex properties. The most simple layer matrix is LC, the layer matrix of *counting*, where $p_v=|H(i)_j|$), simply counts the vertices existing on the *j*th layer located at distance *j* to *i*.

On Layer matrices, an index of *centrality* *C*(**LM**) is calculated; it quantifies the centrality of vertices 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*.

A multi-shell cluster is a part of the 3D-space or of higher dimension spaces and it is called in general a polytope. A 3D-polytope is convex if any of its edges shares no more than two polygons; next, a 4D-polytope is convex if any polygon shares no more than two cells. Each convex 4D-polytope is bounded by a set of 3D cells. If the cells are all Platonic solids of the same type and size, the 4D-polytope is called regular. There are six regular 4D-polytopes, also called polychora and written, using the Schläfli's symbols as: 5-Cell {3,3,3}; 8-Cell {4,3,3}; 16-Cell {3,3,4}; 24-Cell {3,4,3}; 120-Cell {5,3,3} and 600-Cell {3,3,5}. Five of them can be associated to the Platonic solids but the sixth, the 24-cell has no close 3D-equivalent. Among them, 5-Cell and 24-Cell are self-dual while the others are pairs: (8-Cell & 16-Cell); (120-Cell & 600-Cell).

To investigate *n*-dimensional polytopes, the Schläfli formula [9,10] is used

$$\sum_{i=0}^{n-1} (-1)^i f_i = 1 - (-1)^n$$

where f_i are elements of the *f*-vector ($f_0, f_1,\ldots,f_{n-1}$). In case n=4, f_i represent vertices *v*, edges *e*, faces *f* and cells *c*, respectively, while the above sum of figures becomes: $Sum(f_i) = f_0 - f_1 + f_2 - f_3 = 0$. In case n=3, the above is the well-known Euler-Poincaré formula [11]: v-e+f = 2(1-g), with g being the genus [12] (i.e. the number of connections) of the surface in which the graph is embedded. These formulas are useful to check the consistency of the attributed structures.

The article is organized as follows: after the introductory part, some operations on maps are defined to be used in the design of multi-shell clusters. The main clusters based on C_{60} topology, namely C_{750} and C_{810} are discussed in the third section. The forth section deals with the cell duals and their transform in complex clusters. The fifth section gives the equivalence classes of vertices/atoms calculated on two layer matrices of the graphs associated to the studied clusters. Conclusions and references will end the article.

2 Design of multi-shell clusters

Multi-shell clusters herein studied were designed by using map operations, as implemented in our software CVNET [13]. A map M is a discretized surface domain and some operations on maps are known and used to modify a parent map; the parent (marked by a subscript zero) and transformed map parameters refer to regular maps (having all vertices and faces of the same valence/size). The symmetry of parents is preserved by running these operations. For more info, the reader is invited to consult refs. [14-19]. In the following, only the herein used operations are described.

Dual (Du): put a point in the center of each face of the map, next join two such points if their corresponding faces share a common edge. It is the (Poincaré) dual Du(*M*). The vertices of Du(*M*) represent faces in *M* and vice-versa. In the transformed map, the following relations exist: Du(*M*); $v = f_0$; $e = e_0$; $f = v_0$. Dual of the dual returns the original map: Du(Du(*M*)) = *M*. Tetrahedron is self-dual while the other Platonic polyhedra form pairs: Du(Cube) = Octahedron; Du(Dodecahedron) = Icosahedron. It is also known the Petrie dual. Also, a cage-dual is known: in the center of a cage put a point and join two such points if the corresponding cages share a face. If the dual does not account for the infinite face/cage, the dual is called inner dual.

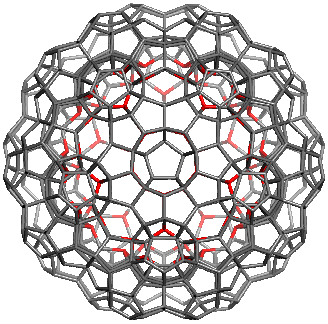
Truncation (Tr): cut off the neighborhood of each vertex by a plane close to the vertex, such that it intersects each edge meeting the vertex. Truncation transformed parameters are:

Tr(*M*); $v = 2e_0 = d_0 v_0$; $e = 3e_0$; $f = f_0 + v_0$. This was the main operation used by Archimedes in building its well-known 13 solids.

Polygonal mapping (P_n): Add a new vertex in the center of each face. Put n-3 points on the boundary edges. Connect the central point with one vertex on each edge (the end points included). Thus, the parent face is covered by triangles (n=3), quadrilaterals (n=4) and pentagons (n=5). The P_3 operation is also called stellation or triangulation. The transformed map parameters are: $P_n(M)$; $v = v_0 + (n-3)e_0 + f_0$; $e = ne_0$; $f = s_0 f_0$.

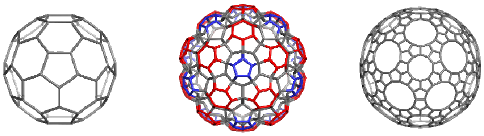
3 C_{60}-related clusters: C_{750} and C_{810}

We start our discussion with introducing two clusters consisting of C_{20} units: C_{750} and C_{810}. They can be designed on $C_{60}(I_h)$ graph using operations on maps, by a procedure recently developed by Diudea [10,20,21]. For this, the following sequence of operations was used: $Trs(P_4(C_{60})).330$; $S_2(C_{60}).420$; $Trs(P_4(C_{60}))@S_2(C_{60}).750$. Structure C_{750} = $C_{60}((C_{20})_{60}).750$ is a "spongy" one, with the central hollow of exact topology of $Trs(P_4(C_{60})).330$.



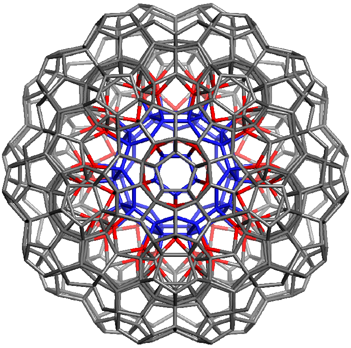
$C_{60}((C_{20})_{60}).750$

$Trs(P_4(C_{60}))@(S_2(C_{60})420).750$



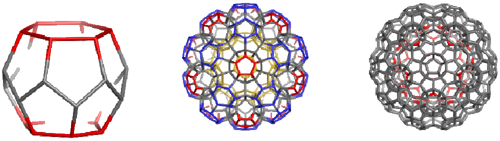
C_{60} **$Trs(P_4(C_{60})).330$** **$S_2(C_{60}).420$**

Figure 1. Multi-shell structures on 750 atoms



$C_{60}@C_{60}((C_{20})_{60}).810$

$C_{60}@((C_{20})_{12};(C_{24})_{20})@(C_{20})_{60}.810$



C_{24} **$C_{60}(@((C_{20})_{12};(C_{24})_{20}).390$** **$C_{60}(Do_{60}).750$**

Figure 2. Multi-shell structures on 810 atoms

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 $C_{60}(I_h)$ [20]. When the hollow $Trs(P_4(C_{60})).330$ is "endohedrally" functionalized (a term taken from nanoscience) by connecting inside the fullerene graph $C_{60}(I_h)$, a double-shell cluster is designed: $C_{60}(@((C_{20})_{12};(C_{24})_{20}).390$. If C_{60} is inserted in C_{750}, the filled structure $C_{810}=C_{60}@C_{750}.810= C_{60}@((C_{20})_{12};(C_{24})_{20})@(C_{20})_{60}.810$ is achieved. The structures involved in the above molecular design are illustrated at the bottom of Figures 1 and 2.

4 Cell dual

Put a vertex in the centre of each cell composing a structure and join such points if the original cells shared a face – thus the cell dual CD is obtained. Vertices of CD represent cells in the original structure and vice-versa. The cell duals for C_{750} and C_{810} are illustrated in

Figure 3. The cell dual of C_{750} is a P-centred-C_{60} cage, $P^{\wedge 60}@C_{60}.61$ (Figure 3, left); if neglect the internal hollow, the dual is simplified to $CD(C_{750})=C_{60}$.

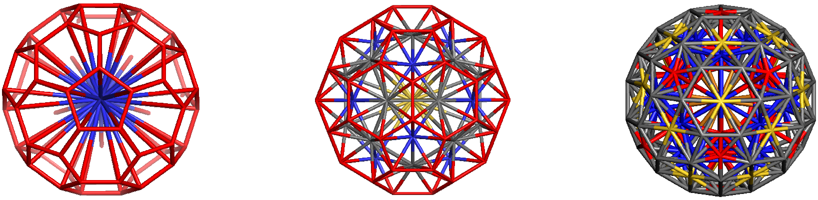


Figure 3. Cell duals: $CD(C_{750})= P^{\wedge 60}@C_{60}.61$(left) ; $CD(C_{810}) = C_{93}= P^{\wedge 32}@Du(C_{60})@C_{60}.93$ (middle) and its stellate $C_{125}=St(P^{\wedge 32}@(Du(C_{60})@C_{60}.93).125= St(P^{\wedge 32}@(St(St(Do)32)93T).125$

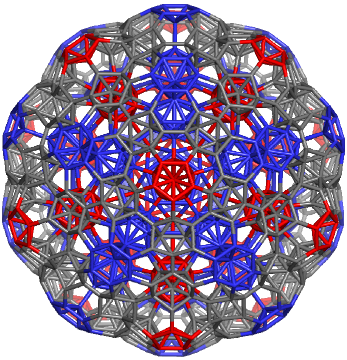
Structures like $IcoP.13=P^{\wedge 12}@Ico.13$ are cell duals of e.g., $CD(C_{130})= CD(C_{20}@(C_{20})_{12})$, or of any structure that joins 12 cells in the I_h symmetry. Note that some 13-atom clusters: MaMb12 or M13, M=Fe, Pd, Ru, Rh show giant magnetic moments [22].

The cell dual $CD(C_{810})$ is a more complicated object (Figure 3, middle); it can be written as $C_{93}=P^{\wedge 32}@Du(C_{60})@C_{60}.93$, where $P^{\wedge 32}$ is the central point of CD, with the superscript (as the power symbol) meaning the connectivity of this point P). Let continue C_{93} by capping/stellating/triangulating the faces f_5 and f_6 of its external shell, having the topology of C_{60}; next, join by a path the two apices of each bipyramid thus formed (and implicitly the central $P^{\wedge 32}$ point), thus obtaining the cluster $C_{125} =St(P^{\wedge 32}@(Du(C_{60})@C_{60}.93).125$ (Figure 3, right). It can also be obtained by the sequence $St(P^{\wedge 32}@(St(St(Do)32)93T).125$, where “T” means the joining of rays of the 93-star to form additional tetrahedra. In the name of structures, the last number is the atoms number; if a structure name is written as a sequence of map operations, the atoms number is preserved, for an ease identification of the steps/shells added. Figure counting for these clusters are given in Table 1. Note that structures having zero sum of their figures represent 4D-objects [10,23].

Truncate now all the vertices of C_{125} cluster to obtain the cluster C_{1208} (Figure 4) . Structure elucidation in such multi-shell clusters is not a trivial task. At least three names can be written for each structure: (i) identify the main substructures, appearing entangled herein; (ii) count all the smallest cells/figures filling the space of cluster and (iii) specify the way of its drawing (by map operations). The endohedral @ symbol was used to suggest the concentric shells, even not clear delimitation of shell is possible in all cases. When the envelope of structure is well-defined (i.e. a fullerene) it is added at the end of name, before the number of atoms.

In case of complex structures, the component figures/shapes are illustrated at the bottom of main structure. A particular mention deserves the cluster C_{84}, related to the celebrate Samson's cluster (on 104 atoms, with 20 atoms located in the center of the truncated tetrahedra TT of C_{84}). It was found in Al-Cu-Li intermetallics [24,25].

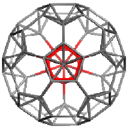
The cluster C_{1208} can be seen as an entanglement of three clusters: C_{244}, C_{84} and C_{100}, each of them being designed by truncation of the corresponding body-centered small clusters (see the bottom structures in Figure 4). We believe that, what we rationalize by geometrical operations used in drawing these objects, to happen in real, at high pressure/high temperature, as in case of synthetic diamond and other diamond like carbon hard phases. Also, it was suggested that domains of the 4D-space coexist with 3D-space in complex minerals.



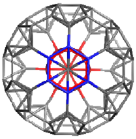
C_{244}@((C_{84})$_{12}$;(C_{100})$_{20}$)@C_{540}(I_h).1208

Du(C_{60})@[(2TT)$_{60}$;(St(Ap_5)$_{12}$;St(Ap_6)$_{20}$]@[(E@TT_5)$_{12}$;(E@TT_6)$_{20}$;(Py_5)$_{12}$;(Py_6)$_{20}$;(J52)$_{60}$)]@C_{540}(I_h).1208

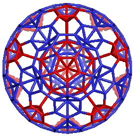
Tr(C_{125}).1208 = C_{1208}



C_{84}=Tr(IcoP).84

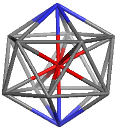


C_{100}=Tr(P@St(Ap_6)).100

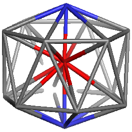


C_{244}=Tr(C_{33}).244

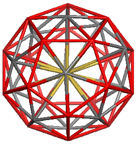
Du(C_{60})@(TT_{12};TT_{20})@C_{180}(I_h).244



P@St(Ap_5).13=IcoP.13



P@St(Ap_6).15



C_{33}=P^^{32}@St(Do).33

Figure 4. C_{1208} and its related structures

Table 1. Euler-Schläfli formula for some of the studied clusters

Cluster	v	e	f_3	f_5	f_6	f	c_1	c_2	c_3	c_4	c_5	c	$\sum f$	M_k;[M]
Du(C_{60}).32	32	90	60	0	0	60	0	0	0	0	0	0	2	$((3^{\wedge 5})_{12};(3^{\wedge 6})_{20})$=St(Do)32
$C_{180}(I_h)$	180	270	0	12	80	92	0	0	0	0	0	0	2	$(5.6^{\wedge 2})60;(6^{\wedge 3})120$
$C_{540}(I_h)$	540	810	0	12	260	272	0	0	0	0	0	0	2	$(5.6^{\wedge 2})60;(6^{\wedge 3})480$
P@St(Ap_5).13	13	42	50	0	0	50	20	0	0	0	1	21	0	T;0;0;0;[St(Ap_5)=Ico.12]
C_{84}	84	192	80	12	50	142	20	12	0	0	2	34	0	TT; Py_5;0;0;[Ico;$C_{60}(I_h)$]
P@St(Ap_6).15	15	50	60	0	0	60	24	0	0	0	1	25	0	T;0;0;0;(St(Ap_6))
C_{100}	100	230	96	12	62	170	24	12	2	0	2	40	0	TT; Py_5;Py_6;0; [St(Ap_6);C72(D_{6d})]
C_{33}	33	122	150	0	0	150	60	0	0	0	1	61	0	T;0;0; 0;(St(Do)32)
Tr(C_{33}).244	244	572	240	12	170	422	60	12	20	0	2	94	0	TT;Py_5;Py_6 ;0; [(Du(C_{60})32;C_{180}]
C_{125}	125	604	870	0	0	870	390	0	0	0	1	391	0	T;0;0;0; (St(C_{60})92)
C_{1208}	1208	3214	1560	12	950	2522	390	24	40	60	2	516	0	TT; (Py_5;St(Ap_5);
	1208	3214	1560	12	890	2462	390	24	40	0	2	456	0	(Py_6;St(Ap_6); J52*; [Du(C_{60})32;C_{540}]

* TT=Truncated Tetraderon; Johnson object J52; Py_k=Pyramid on k- basis; Ap_k=Antiprism on k-basis.

5 CENTRALITY BY LAYER MATRIX OF VERTICES

Centrality of vertices was evaluated by the C-index values, computed on both the layer matrix of rings surrounding each vertex, LR and layer matrix of distance sum LDS. Data are presented in Tables 2 to 5, in descending values of centrality.

Table 2. Symmetry of C_{750}: Automorphism group = $C_2 \times A_5 = I_h$; $|I_h| = 120$.

Class	Centrality signature		No. Vertices	Vertex degree	Atom type
	LR (5;6)	LDS			
1	0.042553749	0.045317	60	4	5^5
2	0.042540566	0.045304	30	4	5^5
3	0.040874143	0.04354	60	3	5^3
4	0.040324963	0.043067	60	4	5^6
5	0.040321521	0.043064	60	4	5^5.6
6	0.040318411	0.043061	60	4	5^5.6
7	0.038098096	0.040826	60	4	5^5
8	0.038077613	0.040805	60	4	5^5
9	0.038052559	0.040778	60	4	5^5
10	0.036396602	0.039075	60	3	5^3
11	0.036389945	0.039038	60	3	5^3
12	0.036339840	0.039019	120	3	5^3

Table 3 Symmetry of C_{810}: Automorphism group $C_2 \times A_5$

Class	Centrality signature		No. Vertices	Vertex degree	Atom type
	LR (5;6)	LDS			
1	0.058307707	0.061944	60	4	5^4.6^2
2	0.053567723	0.057187	60	4	5^6
3	0.052795484	0.056484	60	4	5^6
4	0.052766514	0.056459	30	4	5^6
5	0.048754347	0.052421	60	4	5^5.6
6	0.048749058	0.052417	60	4	5^6
7	0.048732339	0.052403	60	4	5^5.6
8	0.045198403	0.048845	60	4	5^5
9	0.045195080	0.048842	60	4	5^5
10	0.045179071	0.048829	60	4	5^5
11	0.042428574	0.046021	60	3	5^3
12	0.042373172	0.045972	120	3	5^3
13	0.039828281	0.043380	60	3	5^3

Table 4. Symmetry of C_{244}: Automorphism group = $C_2 \times A_5$

Class	Centrality signature LR (3,6)	No. Vertices	Vertex degree	Atom type
1	0.0837441494075746	12	6	3^5.6^10
2	0.0832240289226498	20	7	3^6.5^3.6^9
3	0.0679636030600054	12	6	3^5.6^5
4	0.0675306046381466	20	7	3^6.6^6
5	0.0560796687460724	60	4	3^2.5.6^3
6	0.0557098367436541	60	4	3^2.6^4
7	0.0557092598622740	60	4	3^2.6^4

Table 5. Symmetry of C_{1208}: Automorphism group = $C_2 \times A_5$

Class	Centrality signature LR (3,6)	No. Vertices	Vertex degree	Atom type
1	0.0692967724225917	12	6	3^5.6^10
2	0.0691365154423208	20	7	3^6.5^3.6^9
3	0.0619497820844220	12	6	3^5.5^5.6^5
4	0.0618024674066362	20	7	3^6.5^6.6^6
5	0.0557957706506803	60	6	3^5.5^5.6^5
6	0.0556613506327981	60	6	3^5.5^4.6^6
7	0.0556608929712865	60	6	3^5.5^4.6^6
8	0.0505563870936009	60	6	3^5.5^5.6^5
9	0.0504284365686111	120	6	3^5.5^4.6^6
10	0.0460693873679426	12	6	3^5.5^5.6^5
11	0.0460485352602655	60	6	3^5.5^2.6^5
12	0.0459536270202304	20	7	3^6.5^6.6^6
13	0.0459430688968205	120	6	3^5.5^2.6^5
14	0.0451843719178823	60	5	3^3.5^2.6^4

15	0.0451485654894074	120	5	3^3.5^2.6^4
16	0.0421607708595767	12	6	3^5.6^5
17	0.0421402682758050	60	4	3^2.5.6^3
18	0.0420471142414957	20	7	3^6.6^6
19	0.0420415003258929	120	4	3^2.5.6^3
20	0.0387298595614090	60	4	3^2.5.6^3
21	0.0386382508751928	120	4	3^2.6^4

The same partition of vertices in classes of equivalence resulted according to the two versions of C-index; these classes were confirmed by counting the automorphisms on the adjacency matrix of the molecular graphs by the GAP [26] program.

The graphs associated to the clusters herein discussed were designed by the aid of CVNET [13] while their topology studied by Nano-Studio [27] and Topo Cluj [28] programs.

6 Conclusions

Multi-shell clusters related to the C_{60} fullerene have been designed by using some operations on maps, as implemented in the CVNET software program. Cell duals of some of the studied structures were also built up and next transformed in more complex clusters. Topology of these clusters was evaluated with respect to vertex centrality: the C-index was computed on two types of layer matrices (LR and LDS matrix). Vertices were partitioned in classes of equivalence and ordered according to their centrality. The vertex classification achieved by topological description was confirmed by the automorphisms calculation.

REFERENCES

[1] en.wikipedia.org/wiki/Symmetry.

[2] M. Hargittai, I. Hargittai, *Symmetry through the Eyes of a Chemist*, Springer, Dordrecht, 2010.

[3] M. V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, NOVA, New York, 2002.

[4] T. W. Hungerford, *Algebra*, Reprint of the 1974 original. Graduate Texts in Mathematics, Springer, New York, 1980.

[5] A. R. Ashrafi, F. Kooperazan–Moftakhar, M. V. Diudea, M. Stefu, Mathematics of D_5 network, in: M. V. Diudea, C. L. Nagy (Eds.), *Diamond and Related Nanostructures*, Springer, Dordrecht, 2013, pp. 321.

[6] M. V. Diudea, Molecular topology. 16. Layer matrices in molecular graphs, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1064–1071.

[7] M. V. Diudea, M. Topan, A. Graovac, Molecular topology. 17. Layer matrices of walk degrees, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1072–1078

[8] M. V. Diudea, O. Ursu, Layer matrices and distance property descriptors, *Indian J. Chem.* **42A** (2003) 1283–1294.

[9] L. Schläfli, Theorie der vielfachen Kontinuität Zürcher und Furrer, Zürich, 1901 (Reprinted in: Ludwig Schläfli, 1814–1895, Gesammelte Mathematische Abhandlungen, Band 1, 167–387, Verlag Birkhäuser, Basel, 1950).

[10] M. V. Diudea, Quasicrystals: between Spongy and Full Space Filling, in: M. V. Diudea, C. L. Nagy (Eds.), *Diamond and Related Nanostructures*, Springer, Dordrecht, 2013, pp. 335−385.

[11] L. Euler, Elementa doctrinae solidorum, *Novi. Comm. Acad. Sci. Imp. Petrop.* **4** (1758) 109–160.

[12] F. Harary, *Graph Theory*, Addison–Wesley, Reading, 1969.

[13] M. Stefu, M. V. Diudea, *Cage Versatile_CVNET Sofware*, Babes−Bolyai Univ., Cluj, 2005.

[14] T. Pisanski, M. Randić, Bridges between geometry and graph theory, *Geometry at Work. MAA Notes* **53** (2000)174–194.

[15] M. V. Diudea, Capra−a leapfrog related operation on maps, *Studia Univ. "Babes−Bolyai"* **48** (2003) 3–22.

[16] M. V. Diudea, Nanoporous carbon allotropes by septupling map operations, *J. Chem. Inf. Model.* **45** (2005) 1002–1009.

[17] M. V. Diudea, M. Stefu, P. E. John, A. Graovac, Generalized operations on maps, *Croat. Chem. Acta* **79** (2006) 355–362.

[18] M. V. Diudea, C. L. Nagy, *Periodic Nanostructures*, Springer, Dordrecht, 2007.

[19] M. V. Diudea, *Nanomolecules and Nanostructures − Polynomials and Indices*, Univ. Kragujevac, Kragujevac, 2010.

[20] A. Parvan–Moldovan, F. Kooperazan–Moftakhar, M. V. Diudea, Topological symmetry of multi–shell icosahedral clusters, *Studia Univ. Babes−Bolyai"* **59** (2014) 103−108.

[21] F. Koorepazan–Moftakhar, A. Parvan–Moldovan, M. V. Diudea, Topological symmetry of multi–shell clusters with octahedral symmetry, *Int. J. Chem. Model.* **1** (2015) 231−239.

[22] B. V. Reddy, S. N. Khanna, B. I. Dunlap, Giant magnetic moments in 4*d* clusters, *Phys. Rev. Lett.* **70** (1993) 3323–3326.

[23] V. Y. Shevchenko, G. V. Zhizhin, A. L. Mackay, On the structure of quasicrystals in a higher−dimensional space, in: M. V. Diudea, C. L. Nagy (Eds.), *Diamond and Related Nanostructures*, Springer, Dordrecht, 2013, pp. 311−320.

[24] A. Le Bail, M. Leblanc, M. Audier, Crystalline phases related to the icosahedral AI−Li−Cu phase: a single−crystal X−ray diffraction study of the hexagonal Z−$Al_{59}Cu_5Li_{26}Mg_{10}$ phase, *Acta Cryst.* **B47** (1991) 451−457.

[25] S. Samson, Structural chemistry and molecular biology, in: A. Rich, N. Davidson (Eds.), *Structural Chemistry and Molecular Biology*, Freeman, San Francisco, 1968, pp. 687−717.

[26] *GAP − Groups, Algorithms, Programming − a System for Computational Discrete Algebra*, GAP 4.7.5 release, 2014, http://www.gap−system.org.

[27] C. L. Nagy, M. V. Diudea, *NANO−Studio Software*, Babes−Bolyai Univ., Cluj, 2009.

[28] O. Ursu, M. V. Diudea, *TopoCluj Software*, Babes−Bolyai Univ., Cluj, 2005.