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CENTRALITY OF SOME CUBIC GRAPHS ON 16 VERTICES*

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Abstract . There exist graphs of which all detours are Hamiltonian paths. Such graphs are called by Diudea (*J. Chem. Inf. Comput. Sci.* **1997**, *37*, 1101-1108) *full Hamiltonian detour* FHΔ graphs. These graphs show the maximal value of the Detour index while the minimal value of the Cluj-Detour index. A selected set of cubic graphs on 16 vertices is tested for the distribution of the relative centrality *RC* values, within the Distance, Cluj-Distance and Ring account criteria. The *RC* distribution test is general and can be used in finding the vertex invariant classes and in the characterization of graphs.

Keywords: graph theory, Cluj index, detour index, ring account, relative centrality.

INTRODUCTION

Let $G = (V, E)$ be a connected graph, with no multiple bonds and loops. V is the set of vertices and E is the set of edges in G; $v = |V(G)|$ and $e = |E(G)|$ are their cardinalities.

A *walk w* is an alternating string of vertices and edges: $w_{1,n} = (v_1, e_1, v_2, e_2, ..., v_{n-1}, e_m, v_n)$, with the property that any subsequent pair of vertices represent an edge: $(v_{i-1}, v_i) \in E(G)$. Revisiting of vertices and edges is allowed.[1-4]

The *length* of a walk, $l(w_{1,n}) = |E(w_{1,n})|$ equals the number of its traversed edges. In the above relation $E(w_{1,n})$ is the edge set of the walk $w_{1,n}$. The walk is *closed* if $v_1 = v_n$ and is *open* otherwise.[3,5]

A *path p* is a walk having all its vertices and edges distinct: $v_i \neq v_j$, $(v_{i-1}, v_i) \neq (v_{j-1}, v_j)$ for any $1 \leq i < j \leq n$. As a consequence, revisiting of vertices and edges, as well as branching, is prohibited. The *length* of a path is $l(p_{1,n}) = |E(p_{1,n})| = |V(p_{1,n})| - 1$, with $V(p_{1,n})$ being the vertex set of the path $p_{1,n}$. A closed path is a *cycle* (i.e., *circuit*).

A path is *Hamiltonian* if all the vertices in G are visited at most once: $n = |V(G)|$. If such a path is closed, then it is a *Hamiltonian circuit.*[5]

The *distance* d_{ij}, is the length of a *shortest* path joining vertices v_i and v_j :[3,5]
$d_{ij} = min\ l(p_{ij})$; otherwise $d_{ij} = \infty$. The *set of all distances* (i.e., geodesics) in G is denoted by $D(G)$.

The *detour*, δ_{ij}, is the length of a *longest* path between vertices v_i and v_j :[3,5]
$\delta_{ij} = max\ l(p_{ij})$; otherwise $\delta_{ij} = \infty$. The *set of all detours* in G is denoted by $\Delta(G)$.

In this paper we analyses the equivalence classes of the graphs #1 to #8 (Figure 3) by using three different measures of relative centrality based on Distance (Table 1), Cluj-Distance (Table 2) and Ring-count (Table 3) criteria, as follows.

*This paper is dedicated to the 70th anniversary of Professor Padmakar V. Khadikar, University of Indore, India.

MATERIAL AND METHOD

TOPOLOGICAL MATRICES AND INDICES

The square arrays that collect the distances and detours, in G are called the *Distance* **D** and *Detour* **Δ** matrix**,** respectively: [3,5]

$$[\mathbf{D}(G)]_{i,j} = \begin{cases} \min l(p_{i,j}), \text{if } & i \neq j \\ 0 \text{ if } & i = j \end{cases} \tag{1}$$

$$|\mathbf{\Delta}(G)|_{i,j} = \begin{cases} \max l(p_{i,j}), if & i \neq j \\ 0 \quad if & i = j \end{cases} \tag{2}$$

In words, these matrices collect the number of edges separating the vertices i and j on the shortest and longest path $p_{i,j}$, respectively.

The half sum of entries in the Distance and Detour matrices provide the well-known Wiener index W [6] and its analogue, the detour number w.[7,8]

The *Cluj fragments* represent sets of vertices obeying the relation: [3,5,9]

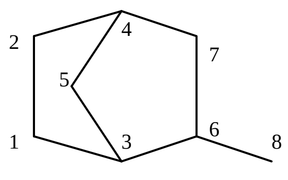
$$CJ_{i,j,p} = \{v | v \in V(G); D_{(G-p)}(i,v) < D_{(G-p)}(j,v)\} \tag{3}$$

The entries in the Cluj matrix **UCJ** are taken, by definition, as the maximum cardinality among all such fragments:

$$[\mathbf{UCJ}]_{\boldsymbol{i,j}} = \max_{p} |CJ_{i,j,p}| \tag{4}$$

It is because, in graphs containing rings, more than one path can join the pair (i, j), thus resulting more than one fragment related to i (with respect to j and path p).

The Cluj matrix is defined by using either *distance* or *detour* concepts: when path p belongs to the set of distances DI(G), the suffix DI is added to the name of matrix, as in UCJDI. When path p belongs to the set of detours DE(G), the suffix is DE. When the matrix symbol is not followed by a suffix, it is by default DI. The Cluj matrices are defined in any graph and, except for some symmetric graphs, are unsymmetric.



G_1

UCJDI

	1	2	3	4	5	6	7	8
1	0	4	2	2	2	2	3	5
2	3	0	2	2	2	3	2	4
3	5	4	0	4	4	4	3	6
4	3	5	3	0	3	3	4	5
5	5	5	2	2	0	4	4	5
6	3	4	3	3	3	0	4	7
7	3	3	2	3	3	3	0	6
8	1	1	1	1	1	1	1	0

UCJDE

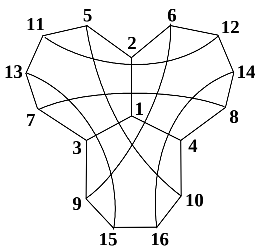
	1	2	3	4	5	6	7	8
1	0	1	1	1	1	2	1	2
2	1	0	1	1	1	1	2	1
3	2	2	0	3	4	2	2	2
4	2	2	2	0	4	2	2	3
5	1	1	1	1	0	1	1	1
6	3	2	2	2	2	0	2	7
7	1	3	1	1	1	1	0	1
8	1	1	1	1	1	1	1	0

Figure 1. Cluj matrices in a ring-containing graph G_1.

An interesting property appears in **UCJDE** version;[10] let consider the vertices 8 (of degree 1) and 5 (of degree 2) of the graph in Figure 1. The vertex 8 is an *external* vertex (with a path ending in it) while the vertex 5 is an *internal* one. An external vertex, like 8, shows all its entries 1 in **UCJDE**.

The same entries are shown by the internal vertex 5. This unusual property we called the *internal ending* of all detours intersecting an *internal endpoint i* in *G*.

There exist graphs with all the vertices internal endpoints and their detours are actually Hamiltonian paths. Such a graph (an example is given in Figure 2) we call *full Hamiltonian detour FHΔ* graph.[10]



$G_{2.}$

DE

0	15	15	15	15	15	15	15	15	15	15	15	15	15	15	15
15	0	15	15	15	15	15	15	15	15	15	15	15	15	15	15
15	15	0	15	15	15	15	15	15	15	15	15	15	15	15	15
15	15	15	0	15	15	15	15	15	15	15	15	15	15	15	15
15	15	15	15	0	15	15	15	15	15	15	15	15	15	15	15
15	15	15	15	15	0	15	15	15	15	15	15	15	15	15	15
15	15	15	15	15	15	0	15	15	15	15	15	15	15	15	15
15	15	15	15	15	15	15	0	15	15	15	15	15	15	15	15
15	15	15	15	15	15	15	15	0	15	15	15	15	15	15	15
15	15	15	15	15	15	15	15	15	0	15	15	15	15	15	15
15	15	15	15	15	15	15	15	15	15	0	15	15	15	15	15
15	15	15	15	15	15	15	15	15	15	15	0	15	15	15	15
15	15	15	15	15	15	15	15	15	15	15	15	0	15	15	15
15	15	15	15	15	15	15	15	15	15	15	15	15	0	15	15
15	15	15	15	15	15	15	15	15	15	15	15	15	15	0	15
15	15	15	15	15	15	15	15	15	15	15	15	15	15	15	0

UCJDE

0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	0	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	0	1	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	0	1	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	0	1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	0	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	0	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	0	1	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	0	1	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	0	1	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	0	1	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	0	1	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	0	1	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	1
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0

Figure 2. Detour and Cluj Detour matrices of a full Hamiltonian detour FHΔ graph G_2.

A FHΔ graph shows all the entries in **UCJDE** equal to 1 and a minimal value for the topological index calculated on this matrix:

$$I(\mathbf{UCJDE}) = \binom{v}{2} = \min \tag{5}$$

In *FHΔ*, the index counts just the number of all vertex pairs, therein joined by Hamiltonian detours.

A related property is shown by the detour matrix.[11,12] There exist *detour saturated graphs*, for which the elements of the detour matrix are maximal. It comes out that their detour index is maximal among the graphs of the same size:

$$w(G) = (n/2)(n-1)^2 = \max \tag{6}$$

FULL HAMILTONIAN DETOUR (*FHΔ*) CUBIC GRAPHS

Figure 3 illustrates a set of distinct cubic graphs, all of them being full Hamiltonian detour graphs, with $I(\mathbf{UCJDE}) = 120$ and w=1800. Note the graph G_2 (see Figure 2) and #8 (Figure 3) are isomorphic. To understand this notion, let us consider two graphs G = (V,E) and G' = (V',E') and a function *f*, *mapping* the vertices of V onto the vertices belonging to the set V', f : V $\rightarrow$ V' . That is, the function *f* makes a one-to-one correspondence between the vertices of the two sets. The two graphs are called *isomorphic*, G ≈ G', if there exists a mapping *f* that preserves adjacency (*i.e.*, if $(i,j) \in$ E, then $(f(i), f(j)) \in$ E'). The isomorphism of *G* with itself is called an automorphism. It is demonstrated that all the automorphisms of *G* form a group, *Aut*(G).[3,5]

In the chemical field, the isomorphism search could answer to the question if two molecular graphs represent or not one and the same chemical compound. Two isomorphic graphs will show the same topological indices, so that they cannot be distinguished by topological descriptors.

The symmetry of a graph is often called a topological symmetry; it is defined in terms of *connectivity*, as a constitutive principle of molecules and expresses equivalence relationships among elements of the graph: vertices, bonds, faces or larger subgraphs.[5]

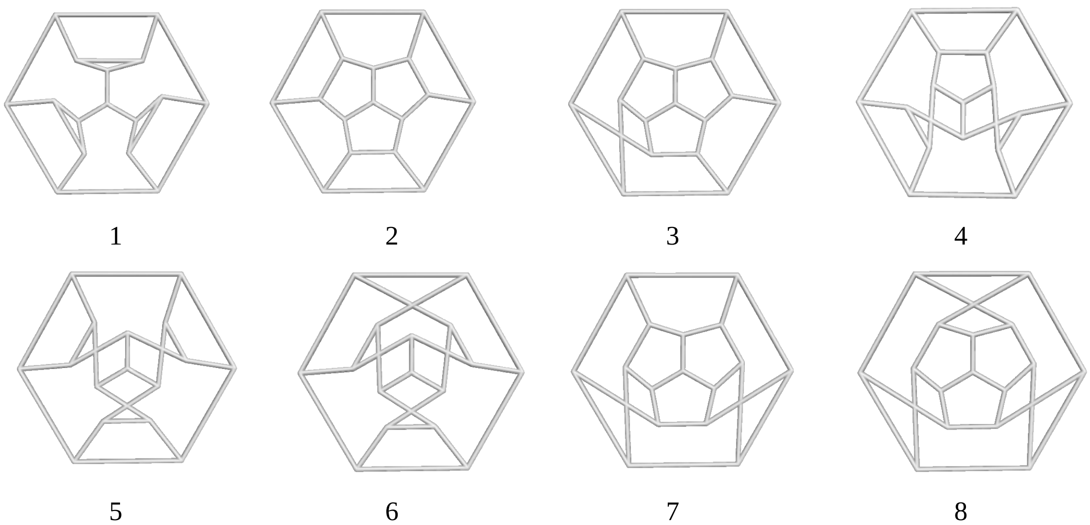


Figure3. Full Hamiltonian Detour $FH\Delta$ graphs (of degree 3) on 16 vertices, with rings from 3 to 7 vertices/atoms.

The topological symmetry[5,13] does not fully determine the molecular geometry; it does not need to be the same as the molecular point group symmetry. However, it does represent the maximal symmetry which the geometrical realization of a given topological structure may posses.[14] Given a graph G=(V, E) and a group Aut(G),[15-17] we call two vertices, i, $j \in$V *equivalent* if there is a group element, aut(v_i)$\in$Aut(G), such that j aut(v_i) i. The set of all vertices j (obeying the *equivalence relation*) is called i's class of equivalence. Two vertices i and j, showing the same vertex invariant $In_i = In_j$, belong to the same *invariant class IC*. The process of vertex partitioning in ICs leads to m classes, with v_1, v_2,...v_m vertices in each class. Note that invariant-based partitioning 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.[3,5]

In this paper we look for equivalence classes of the graphs #1 to #8 (Figure 3), as given by using the centrality functions (7, 8): [3,5,18]

$$C(\mathbf{LM})_i = \left[\sum_{k=1}^{ecc_i} \left(\left[\mathbf{LM}\right]_{ik}^{2k} \right)^{1/(ecc_i)^2} \right]^{-1} \tag{7}$$

$$C(\mathbf{LM}) = \sum_i C(\mathbf{LM})_i \tag{8}$$

This index allows the finding of the graph center and provides an ordering of the graph vertices according to their centrality. It can also be calculated by using the Shell matrices **ShM** instead of **LM** ones.[18]

The entries in the layer matrix (of vertex property) **LM**, are defined as[5,19,20]

$$\left[\mathbf{LM}\right]_{i,k} = \sum_{v | d_{i,v}=k} p_v \tag{9}$$

Layer matrix is a collection of the above defined entries:

$$\mathbf{LM}(G)=\left\{ [\mathbf{LM}]_{i,k};\, i\in V(G);\, k\in[0,1,..,d(G)] \right\} \tag{10}$$

with $d(G)$ being the diameter of the graph (*i.e.*, the largest distance in G). Any atomic/vertex property can be considered as p_i. More over, any square matrix **M** can be taken as *info matrix*, *i.e.*, the matrix supplying local/vertex properties as row sum *RS*, column sum *CS*. The zero column is just the column of vertex properties $[\mathbf{LM}]_{i,0}=p_i$. When the vertex property is 1 (i.e., the counting property), the **LM** matrix will be **LC** (the Layer matrix of Counting).

Define the entries in the shell matrix **ShM** (of pair vertex property) as[5,18]

$$[\mathbf{ShM}]_{i,k}=\sum_{v|d_{i,v}=k}[\mathbf{M}]_{i,v} \tag{11}$$

The shell matrix is a collection of the above defined entries:

$$\mathbf{ShM}(G)=\left\{ [\mathbf{ShM}]_{i,k};\, i\in \mathrm{V}(G);\, k\in[0,1,..,d(G)] \right\} \tag{12}$$

A shell matrix **ShM**(G), will partition the entries of the square matrix according to the vertex (distance) partitions in the graph. It represents a true decomposition of the property collected by the info square matrix according to the contributions brought by pair vertices pertaining to shells located at distance k around each vertex. The zero column entries $[\mathbf{ShM}]_{i,0}$ are just the diagonal entries in the info matrix. The properties of layer/shell matrices **LM**/**ShM** have been discussed elsewhere.[18-20]

In the following, we will focus attention not on the vertex centrality ordering (for this subject, the reader is invited to consult our monographs[3,5]) but to a *relative centralily*, obtained by normalizing with the highest value of centrality function in a graph and next by the number of vertices in G:

$$RC(\mathbf{LM})_i=C(\mathbf{LM})_i\,/\max C(\mathbf{LM})_i \tag{13}$$

$$RC(\mathbf{LM})=\sum\nolimits_i RC(\mathbf{LM})_i/|V(G)| \tag{14}$$

This relative centrality gives account of the *deviation to the maximum centrality*, equaling 1 in case all the vertices are centers of the graph (*e.g.*, the case of simple cycles).

RESULTS AND DISCUSSION

In the present paper, the values of RC for the graphs in Figure 3 are calculated within the Distance (Table 1), Cluj-Distance (Table 2) and Ring-count (Table 3) criteria, as follows.

In the Distance criterion, **D** matrix is taken as **LD** (i.e., the row sums in **D** matrix become the zero-column in **LM**=**LD**); In the Cluj matrix criterion, the matrix **UCJDI** isoperated by Diudea's Shell-operator.[18]

In the Ring-count criterion, the entries in the layer matrix of rings **LR** is calculated as:

$$[\mathbf{LR}]_{i,k}=R(i)_k \tag{15}$$

with $R(i)_k$ is the number of rings of length k passing through vertex i, while the whole **LR** matrix is the collection of these entries, up to a chosen length (an upper bond is v=|V(G)|:

$$\mathbf{LR}(G) = \left\{ [\mathbf{LR}]_{i,k}; i \in \mathrm{V}(G); k = chosen \right\} \quad (16)$$

Table 1. Relative centrality, local (RC_i) and global (RC) values, no. of invariant classes IC and their population Pop (no. of vertices) for the graphs #1 to #8; I=C(**LD**).

#	1	2	3	4	5	6	7	8
1	0.6166	1	1	1	0.9993	0.9982	1	1
2	1	0.6390	0.6381	0.7064	1	1	0.7060	1
3	0.6166	0.6277	0.7011	0.6915	0.9447	0.6949	0.7061	1
4	0.6166	0.6277	0.7011	0.6296	0.9447	0.9975	0.9986	1
5	0.5385	0.6303	0.7018	0.6963	0.9481	1	1	1
6	0.5385	0.6390	0.7084	0.7064	1	0.9955	1	1
7	0.6193	0.6277	0.6313	0.6915	0.9447	0.9984	0.7060	1
8	0.6193	0.6303	0.7080	0.6963	0.9481	0.7025	0.7061	1
9	0.5385	0.6390	0.7084	0.9990	1	1	0.7060	1
10	0.5385	0.6277	0.6313	0.6945	0.9447	0.9975	0.9986	1
11	0.6193	0.6303	0.7018	0.6982	0.9481	0.9809	0.9982	1
12	0.6193	0.6303	0.7080	0.6929	0.9481	0.9809	0.9982	1
13	0.5385	0.6277	0.7075	0.6945	0.9447	0.6949	0.7061	1
14	0.5385	0.6277	0.7075	0.6296	0.9447	0.9984	0.7060	1
15	0.6193	0.6303	0.6943	0.6929	0.9481	1	1	1
16	0.6193	0.6303	0.6943	0.6982	0.9481	0.7025	0.7061	1
Sum	9.7971	10.4647	11.3426	11.6179	15.3564	14.7423	13.6423	16
RC	**0.6123**	**0.6540**	**0.7089**	**0.7261**	**0.9598**	**0.9214**	**0.8526**	**1**
IC	4	4	9	9	4	8	5	1
Pop	$1,3,(6)_2$	$1,3,(6)_2$	$(1)_2,(2)_7$	$(1)_2,(2)_7$	$1,3,(6)_2$	$(1)_2,(2)_5,4$	$(2)_2,(4)_3$	16

Table 2. Relative centrality, local(RC_i) and global (RC) values, no. of invariant classes IC and their population Pop (no. of vertices) for the graphs #1 to #8; I=C(**ShUCJDI**).

#	1	2	3	4	5	6	7	8
1	1	1	1	1	0.9720	0.9836	0.9969	0.9676
2	0.7512	0.7059	0.7213	0.7560	0.9598	0.9680	0.7725	1
3	0.7512	0.7239	0.7818	0.7637	1	0.7717	0.7763	0.9863
4	0.7512	0.7239	0.7818	0.7259	1	0.9829	1	0.9863
5	0.6659	0.7255	0.7702	0.7652	0.9825	0.9628	0.9969	0.9949
6	0.6659	0.7059	0.7733	0.7560	0.9598	0.9494	0.9969	1
7	0.6882	0.7239	0.7368	0.7637	1	0.9613	0.7725	0.9863
8	0.6882	0.7255	0.7935	0.7652	0.9825	0.7383	0.7763	0.9949
9	0.6659	0.7059	0.7733	0.9877	0.9598	0.9680	0.7725	1
10	0.6659	0.7239	0.7368	0.7629	1	0.9829	1	0.9863
11	0.6882	0.7255	0.7702	0.7952	0.9825	1	0.9992	0.9949
12	0.6882	0.7255	0.7935	0.7860	0.9825	1	0.9992	0.9949
13	0.6659	0.7239	0.7780	0.7629	1	0.7717	0.7763	0.9863
14	0.6659	0.7239	0.7780	0.7259	1	0.9613	0.7725	0.9863
15	0.6882	0.7255	0.8028	0.7860	0.9825	0.9628	0.9969	0.9949
16	0.6882	0.7255	0.8028	0.7952	0.9825	0.7383	0.7763	0.9949
Sum	10.3780	11.8141	12.5939	12.6975	15.7465	14.7033	14.1814	15.8549
RC	**0.6486**	**0.7384**	**0.7871**	**0.7936**	**0.9842**	**0.9190**	**0.8863**	**0.9909**
IC	4	4	9	9	4	9	5	4
Pop	$1,3,(6)_2$	$1,3,(6)_2$	$(1)_2,(2)_7$	$(1)_2,(2)_7$	$1,3,(6)_2$	$(1)_2,(2)_7$	$(2)_2,(4)_3$	$1,3,(6)_2$

Table 3. Relative centrality, local(RC_i) and global (RC) values, no. of invariant classes IC and their population Pop (no. of vertices) for the graphs #1 to #8; I=C(**LCy**).

#	1	2	3	4	5	6	7	8
1	1	0.934525	1	0.966019	0.972109	0.964336	1	0.930743
2	0.802226	0.953048	0.996252	0.989216	0.988886	0.936367	0.964186	0.987698
3	1	1	0.958911	0.998263	1	0.994514	0.953163	0.976554
4	1	1	0.958911	0.99658	1	0.987293	0.96221	0.976554
5	0.967995	0.986962	0.942862	0.990571	0.999659	0.970432	0.97435	1
6	0.967995	0.953048	0.96814	0.989216	0.988886	0.923571	1	0.987698
7	0.873761	1	0.973478	0.998263	1	0.942381	0.964186	0.976554
8	0.873761	0.986962	0.916903	0.990571	0.999659	0.955126	0.953163	1
9	0.967995	0.953048	0.96814	0.929073	0.988886	0.936367	0.964186	0.987698
10	0.967995	1	0.973478	0.983684	1	0.987293	0.96221	0.976554
11	0.873761	0.986962	0.942862	1	0.999659	1	0.875436	1
12	0.873761	0.986962	0.916903	0.972476	0.999659	1	0.875436	1
13	0.967995	1	0.991259	0.983684	1	0.994514	0.953163	0.976554
14	0.967995	1	0.991259	0.99658	1	0.942381	0.964186	0.976554
15	0.873761	0.986962	0.970855	0.972476	0.999659	0.970432	0.97435	1
16	0.873761	0.986962	0.970855	1	0.999659	0.955126	0.953163	1
Sum	14.85276	15.71544	15.44107	15.75667	15.93672	15.46013	15.29339	15.75316
RC	**0.928298**	**0.982215**	**0.965067**	**0.984792**	**0.996045**	**0.966258**	**0.955837**	**0.984573**
IC	4	4	9	9	4	9	6	4
Pop	$1,3,(6)_2$	$1,3,(6)_2$	$(1)_2,(2)_7$	$(1)_2,(2)_7$	$1,3,(6)_2$	$(1)_2,(2)_7$	$(2)_4,(4)_2$	$1,3,(6)_2$

From Table 1, one can see that the graph #8 appears as an "all central vertex" ACV graph (like the simple cycles), in the Distance-sum criterion. The more discriminant Cluj matrix[9] succeeded in separating the invariant classes *IC* of #8 (Table 2, last column). According to the relative centrality global value *RC*, #8 remain, by this criterion, the closest structure to the ACV status (RC=0.9909), followed by #5 (RC=0.9842).[21]

However, changing the criterion to the Ring counting, the largest RC value is shown by #5 (RC=0.9960). If we look for a maximal centrality, different distribution can be seen.

The invariant classes IC are found the same in the three criteria, excepting those for structures #6 to #8.

Note, the graphs in Figure 3 have been selected (randomly, except #8 and #2) from a large pool of FHΔ, among the possible cubic graphs (*i.e.*, graphs of uniform vertex degree 3) on 16 vertices. The study on the whole pool of cubic graphs on 16 vertices, including the automorphism group analysis, is in progress at the TOPO Group Cluj and will be published in a future article.

CONCLUSIONS

It was shown that the graphs, with all their detours being Hamiltonian paths, called *full Hamiltonian detour* FHΔ graphs, show the maximal value of the Detour index and the minimal value of the Cluj-Detour index. In the set of cubic graphs on 16 vertices herein tested for the distribution of the relative centrality *RC* values, the three criteria: Distance, Cluj-Distance and Ring account, found the same vertex invariant classes IC, excepting the last three structures. The most discriminant appeared the Cluj matrix- and ring-based criteria. The RC distribution test is general and can be used in the characterization of any graphs.

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