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ORIGINAL PAPER

Subgraphs of pair vertices

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Abstract Subgraphs obtained by applying several fragmentation criteria are investigated. Two well known criteria (Szeged and Cluj), and two new others are defined and characterized. An example is given for the discussed procedures. The matrix and polynomial representations of vertices composing each type of subgraphs were also given. Analytical formulas for the polynomials of several classes of graphs are derived. The newly introduced subgraphs/fragments, called MaxF and CMaxF, appear to have interesting properties, which are demonstrated.

Keywords Subgraphs · Chemical graph theory · Graph polynomials

1 Definition of fragments

Let V be a set and $E \subseteq V \times V$ a subset of the Cartesian product [1,2] V × V. Then $G = (V, E)$ be an un-oriented graph, with $V(G)$ the set of vertices and E(G) the set of edges. A graph is connected if there is a path from one to any other vertex in G [3,4].

Let denote by $\mathbf{D}(G)$ the distance matrix [2] of G. In terms of distance matrix, the connectivity of G is written as: $D(G)_{i,j} < \infty$ for any $i, j \in V(G)$.

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The *Szeged fragmentation criterion* was introduced by Gutman [5]. Szeged subgraphs can be defined as follows:

$$SzF(G)_{i,j} = \{V(SzF(G)_{i,j}), E(SzF(G)_{i,j})\} \tag{1}$$

$$V(SzF(G)_{i,j}) = \{s \in V(G) | D(G)_{s,i} < D(G)_{s,j}\} \tag{2}$$

$$E(SzF(G)_{i,j}) = \{(s,t) \in E(G) | s,t \in V(SzF(G)_{i,j})\} \tag{3}$$

The Szeged set $SzF(G)_{i,j}$ is a connected subgraph (the set results from a geodesic operator).

Cluj fragmentation criterion was introduced by Diudea et al. [6–10]. The Cluj subgraphs are defined on a path $p(i, j)$ separating the vertices i and j:

$$CjF(G)_{i,j,p} = SzF(G_p)_{i,j} \tag{4}$$

where G_p is obtained from G by deleting the path p with exception of its endpoints. The Cluj fragments are also connected subgraphs [2].

A minimal subgraph of G can be defined as follows:

$$MinF(G)_{i,j} = (\{i\}, \emptyset) \tag{5}$$

The above definition of minimal subgraphs is a trivial one. Such a subgraph always contains one vertex, the vertex i.

A maximal connected subgraph of G, containing the vertex i but not the vertex j, we denote here by $MaxF(G)_{i,j}$. Such maximal connected subgraphs can be constructed by using a temporary graph, $(VTemp(G)_{i,j}, ETemp(G)_{i,j})$, to be defined below, which is a disconnected graph:

$$VTemp(G)_{i,j} = \{s \in V(G) | s \neq j\}, ETemp(G)_{i,j} = \{(u,v) \in E(G) | u, v \neq j\} \tag{6}$$

The $V(MaxF(G)_{i,j})$ and $E(MaxF(G)_{i,j})$ sets are defined as follows:

$$V(MaxF(G)_{i,j}) = \{s \in VTemp(G)_{i,j} | D(VTemp(G)_{i,j})_{s,i} < \infty\} \tag{7}$$

$$E(MaxF(G)_{i,j}) = \{(s,t) \in E(G) | s,t \in V(MaxF(G)_{i,j})\} \tag{8}$$

Let now construct the complementary subgraph $CMaxF(G)_{i,j}$ of maximal connected subgraph $MaxF(G)_{i,j}$ with respect to the graph G:

$$CMaxF(G)_{i,j} = (V(CMaxF(G)_{i,j}), E(CMaxF(G)_{i,j})) \tag{9}$$

$$V(CMaxF(G)_{i,j}) = \{s \in V(G) | s \notin V(MaxF(G)_{i,j})\} \tag{10}$$

$$E(CMaxF(G)_{i,j}) = \{(s,t) \in E(G) | s,t \in V(CMaxF(G)_{i,j})\} \tag{11}$$

The new substructure $CMaxF(G)_{i,j}$ is, in general, a smaller one. Rarely it has more than one element (one vertex, the vertex j). However, it differs from $MinF(G)_{i,j} = (\{i\}, \emptyset)$, as it is shown in following example:

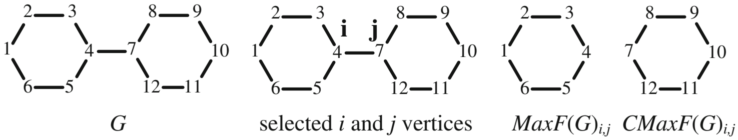

Fig. 1 $MaxF(G)$ and $CMaxF(G)$ subgraph definition

Figure 1 illustrates a graph G, and the way of generating the fragments $MaxF(G)_{i,j}$ and $CMaxF(G)_{i,j}$. As can be seen, $G \neq MaxF(G)_{i,j} \cup CMaxF(G)_{i,j}$ (by the edge (i, j)).

2 Matrices derived from fragmentation

Let us present the matrix representation [3,4,10] of subgraphs generated by the above four fragmentation criteria.

The entries in matrices [**MaxF**], [**CMaxF**], and [**SZ**] matrix [11] are similar and represent the vertex cardinality of subgraphs, viewed as sets of vertices:

$$[\mathbf{M}]_{i,j} = |\mathbf{M}(G)_{i,j}|, \ \ where\ \mathbf{M} \in \{\mathbf{MaxF}, \mathbf{CMaxF}, \mathbf{SZ}\} \tag{12}$$

while for **CJ** matrix (according to Ref. [6,7]) is:

$$[\mathbf{CJ}]_{i,j} = max\{|CJF(G)_{i,j,p}|;\ \ p \in P(G)_{i,j}\} \tag{13}$$

Tables 1–4 give examples of the above matrices in case of graph G. Note that the above matrices are unsymmetric (exception some symmetric graphs). More about the **SZ** and **CJ** matrices the reader can find in Ref. [4,10].

Table 1 Matrix **MaxF** for the graph G

MaxF	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	11	11	5	11	11	6	11	11	11	11	11	110
2	11	0	11	5	11	11	6	11	11	11	11	11	110
3	11	11	0	5	11	11	6	11	11	11	11	11	110
4	11	11	11	0	11	11	6	11	11	11	11	11	116
5	11	11	11	5	0	11	6	11	11	11	11	11	110
6	11	11	11	5	11	0	6	11	11	11	11	11	110
7	11	11	11	6	11	11	0	11	11	11	11	11	116
8	11	11	11	6	11	11	5	0	11	11	11	11	110
9	11	11	11	6	11	11	5	11	0	11	11	11	110
10	11	11	11	6	11	11	5	11	11	0	11	11	110
11	11	11	11	6	11	11	5	11	11	11	0	11	110
12	11	11	11	6	11	11	5	11	11	11	11	0	110
	121	121	121	61	121	121	61	121	121	121	121	121	1,332

$MaxF(G, x) = 10x^5 + 12x^6 + 110x^{11}$; $D1|_{x=1} = 1{,}332$

Table 2 Matrix **CMaxF** for the graph G

CMaxF	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	1	1	7	1	1	6	1	1	1	1	1	22
2	1	0	1	7	1	1	6	1	1	1	1	1	22
3	1	1	0	7	1	1	6	1	1	1	1	1	22
4	1	1	1	0	1	1	6	1	1	1	1	1	16
5	1	1	1	7	0	1	6	1	1	1	1	1	22
6	1	1	1	7	1	0	6	1	1	1	1	1	22
7	1	1	1	6	1	1	0	1	1	1	1	1	16
8	1	1	1	6	1	1	7	0	1	1	1	1	22
9	1	1	1	6	1	1	7	1	0	1	1	1	22
10	1	1	1	6	1	1	7	1	1	0	1	1	22
11	1	1	1	6	1	1	7	1	1	1	0	1	22
12	1	1	1	6	1	1	7	1	1	1	1	0	22
	11	11	11	71	11	11	71	11	11	11	11	11	252

$CMaxF(G, x) = 110x + 12x^6 + 10x^7$; $D1|_{x=1} = 252$

Table 3 Matrix **SZ** for the graph G

SZ	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	3	2	3	2	3	3	5	5	6	5	5	42
2	9	0	3	2	3	2	4	4	6	6	6	4	49
3	8	9	0	3	2	9	3	6	6	7	6	6	65
4	9	8	9	0	9	8	6	6	8	7	8	6	84
5	8	9	2	3	0	9	3	6	6	7	6	6	65
6	9	2	3	2	3	0	4	4	6	6	6	4	49
7	7	8	6	6	6	8	0	9	8	9	8	9	84
8	7	6	6	3	6	6	3	0	9	8	9	2	65
9	6	6	4	4	4	6	2	3	0	9	2	3	49
10	6	5	5	3	5	5	3	2	3	0	3	2	42
11	6	6	4	4	4	6	2	3	2	9	0	3	49
12	7	6	6	3	6	6	3	2	9	8	9	0	65
	82	68	50	36	50	68	36	50	68	82	68	50	708

$SZ(G, x) = 16x^2 + 24x^3 + 12x^4 + 8x^5 + 36x^6 + 6x^7 + 12x^8 + 18x^9$; $D1|_{x=1} = 708$

3 Polynomial representation of fragmentations

A counting polynomial [12–14] is a representation of a sequence of numbers, with the exponents showing the extent of partitions $p(G), \cup p(G) = P(G)$ of a graph property $P(G)$ while the coefficients $m(G, k)$ are related to the occurrence of partitions of extent k.

$$P(G, x) = \sum_k m(G, k) \cdot x^k \tag{14}$$

The coefficients of counting polynomials related to the above fragmentations can be obtained from the corresponding matrices, by counting of the occurrence of their entries. For the graph G, the related polynomials are given under each of the

Table 4 Matrix **CJ** for the graph G

CJ	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	3	2	2	2	3	3	3	3	3	3	3	30
2	9	0	3	2	2	2	4	4	4	4	4	4	42
3	8	9	0	3	2	8	5	5	5	5	5	5	60
4	8	8	9	0	9	8	6	6	6	6	6	6	78
5	8	8	2	3	0	9	5	5	5	5	5	5	60
6	9	2	2	2	3	0	4	4	4	4	4	4	42
7	6	6	6	6	6	6	0	9	8	8	8	9	78
8	5	5	5	5	5	5	3	0	9	8	8	2	60
9	4	4	4	4	4	4	2	3	0	9	2	2	42
10	3	3	3	3	3	3	2	2	3	0	3	2	30
11	4	4	4	4	4	4	2	2	2	9	0	3	42
12	5	5	5	5	5	5	3	2	8	8	9	0	60
	69	57	45	39	45	57	39	45	57	69	57	45	624

$CJ(G, x) = 22x^2 + 24x^3 + 24x^4 + 24x^5 + 12x^6 + 14x^8 + 12x^9$; $D1|_{x=1} = 624$

Tables 1–4. It is easily seen that the first derivative, in x= 1, equals the sum of entries in the corresponding matrices.

The polynomial representation is useful in partitioning a graph property in view of weighting the subgraph contributions by physico-chemical characteristics of the vertices/atoms composing a molecular graph.

Table 5 lists the formulas for calculating the discussed polynomials for several classes of graphs.

4 Properties of subgraphs generated by fragmentation

Theorem 1 *In a not empty graph G, the following relations hold:*

$$1 = n_{MinF} \le n_{CJF}, n_{SZF} \le n_{MaxF} \le n_G;\ \text{where } n_A = |A| \tag{15}$$

Demonstration. By definition, it is immediate that $1 = n_{MinF}$; next, $n_{MinF} \le n_{CJF}, n_{SZF}$ comes from: $\{i\} \subset V(SZF(G)_{i,j})$ and $V(CJF(G)_{i,j}$. The relation n_{CJF}, $n_{SZF} \le n_{MaxF}$ is true because both Szeged and Cluj fragments collect all vertices lying closer to i than to j, excluding the vertices equidistant to i and j whereas MaxF criterion excludes, at the start, only the j vertex, and next all vertices, which become non-connected to i. These vertices are also not found in $V(CjF(G)_{i,j,p})$ and $V(SzF(G)_{i,j})$, which are both connected subgraphs containing the vertex i. The Cluj fragment excludes, in addition, the vertices belonging to the path $p_{i,j}$. The last inequality is even more immediate, as long as $V(MaxF(G)_{i,j})$ is constructed on the vertices of V(G).

Even if $n_{CJF} \le n_{SZF}$, for any p from i to j, the inclusion $V(CjF(G)_{i,j,p}) \subseteq V(SzF(G)_{i,j})$ or its reverse is false, in general.

The following example (Fig. 2) illustrates the above results.

Table 5 Formulas for polynomials of several classes of graphs

	G	Polynomial
1	Star $S_{1,n}$	$\mathrm{MaxF}(G, x) = (n+1)x^0 + nx^1 + n^2x^n$ $\mathrm{CMaxF}(G, x) = \mathrm{SZ}(G, x) = \mathrm{CJ}(G, x) = (n+1)x^0 + n^2x^1 + nx^n$
2	Path P_n	$\mathrm{MaxF}(G, x) = nx^0 + 2\sum_{1\le k<n} kx^k$ $\mathrm{CMaxF}(G, x) = \mathrm{CJ}(G, x) = nx^0 + 2\sum_{1\le k<n}(n-k)x^k$ $\mathrm{SZ}(G, x) = nx^0 + 4\sum_{1\le k\le(2n-1+(-1)^n)/4} kx^k$ $+2\sum_{1\le k\le(2n-3+(-1)^n)/4}(2k-1)x^{n+1-k}$
3	Complete K_n	$\mathrm{MaxF}(G, x) = nx^0 + n(n\text{-}1)x^{n-1}$ $\mathrm{CMaxF}(G, x) = \mathrm{CJ}(G, x) = \mathrm{SZ}(G, x) = nx^0 + n(n-1)x$
4	Dendrimers[a] $D_{f,s}$	$\mathrm{MaxF}(G, x) = \frac{f(f-1)^s-2}{f-2}x^0 + f\sum_{0\le k<s}(f-1)^{s-k-1}\frac{(f-1)^{k+1}-1}{f-2}x^{\frac{(f-1)^{k+1}-1}{f-2}}$ $+f\sum_{0\le k<s}(f-1)^{s-k-1}\frac{f(f-1)^s-(f-1)^{k+1}-1}{f-2}x^{\frac{f(f-1)^s-(f-1)^{k+1}-1}{f-2}}$ $\mathrm{CMaxF}(G, x) = \frac{f(f-1)^s-2}{f-2}x^0 + f\sum_{0\le k<s}(f-1)^{s-k-1}\frac{f(f-1)^s-(f-1)^{k+1}-1}{f-2}x^{\frac{(f-1)^{k+1}-1}{f-2}}$ $+f\sum_{0\le k<s}(f-1)^{s-k-1}\frac{(f-1)^{k+1}-1}{f-2}x^{\frac{f(f-1)^s-(f-1)^{k+1}-1}{f-2}} = \mathrm{CJ}(G, x)$ $\mathrm{SZ}(G, x) = \frac{f(f-1)^s-2}{f-2}x^0$ $+f\sum_{0<k\le s}\frac{(f-1)^{s-k}}{f-2}\left(\left((f-1)^{2k-1}\right)x^{\frac{(f-1)^k-1}{f-2}}\right.$ $\left.+\left((f-1)^{2k-1}-1\right)x^{\frac{f(f-1)^s-(f-1)^k-1}{f-2}}\right)$

[a] s letter in the dendrimers[15] formula stands for the layer; in layer "0" there is 1 atom, in layer "1" there are f atoms (counting the number of atoms: $n = f + 1$)

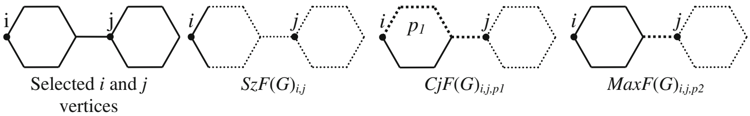

Fig. 2 Examples of fragments $MaxF(G)$, $SzF(G)_{i,j}$ and $CjF(G)_{i,j,p}$ subgraphs

The $MaxF(G)_{i,j}$ is a connected subgraph (let's denote subgraph by "$\prec$") of G, by construction:

$$MaxF(G)_{i,j} \prec G \tag{16}$$

Theorem 2 *$CMaxF(G)_{i,j}$ is a connected subgraph of G:*

$$CMaxF(G)_{i,j} \prec G \tag{17}$$

Demonstration. Clearly, $CMaxF(G)_{i,j}$ is a subgraph of G. All its vertices and edges belong to G. The difficulty is to prove its connectivity. Suppose there exists a vertex k not connected in any way with the vertex j (i.e., $D(CMaxF(G)_{i,j})_{k,j} = \infty$). But k belongs to G, thereby $D(G)_{k,i} < \infty$, and also $D(G)_{k,j} < \infty$. We can assume there is a path from k to i: $k = x_0, x_1, \ldots, x_n = i$. If none of its vertices $x_1, \ldots, x_{n-1}$ is j we goes to a contradiction because, in this case, our vertex k is in the wrong place ($CMaxF(G)_{i,j}$); its place must be $MaxF(G)_{i,j}$. If one of the vertices $x_1, \ldots, x_{n-1}$ is j then we have an interesting path: $k = x_0, \ldots x_{m-2}, x_{m-1}, x_m = j, x_{m+1} \ldots x_n = i$. If $(x_{m-1}, x_m) \in E(G)$, and $x_{m-1}, x_m \in V(CMaxF(G)_{i,j})$ then (by definition of $CMaxF(G)_{i,j}$) it results that $(x_{m-1}, x_m) \in E(CMaxF(G)_{i,j})$; thus, x_{m-1} *is connected* to $x_m = j$ in $CMaxF(G)_{i,j}$. By recursion to all the vertices $x_{m-2}, \ldots, x_0 = k$ of our path, we conclude that k *is connected to* j.

Theorem 3 *In any connected graph, with more than two vertices, the following relations hold:*

$$SzF(G)_{i,j}, CjF(G)_{i,j,p} \prec MaxF(G)_{i,j} \prec G \tag{18}$$

Demonstration. Demonstration comes from the definitions of the three fragments. The fact that G is the biggest graph is beyond dispute. If either $SzF(G)_{i,j}$, or $CjF(G)_{i,j,p}$ has an edge (s, t), then using a similar judgment as for (17), also $MaxF(G)_{i,j}$ must have it; also (even more simple is) for a vertex. An interesting property is revealed by the graph polynomial of *MaxF* fragmentation, by the example for the graph G:

$$MaxF(G, x) = 2 \cdot 5 \cdot x^5 + 2 \cdot 6 \cdot x^6 + 10 \cdot 11 \cdot x^{11} \tag{19}$$

Equation 19 shows that:

Theorem 4 *The number of occurrences of a given size subgraph, generated by MaxF criterion applied to a graph G, equals the number of vertices consisting the subgraph.*

Demonstration. A subgraph $MaxF(G)_{i,j}$, with vertex cardinality $n_{i,j} = |MaxF(G)_{i,j}|$ refers to one and the same reference cut-point j, and by construction, *one fragment for each vertex* $i = 1, 2, \ldots, n_{i,j}$ can be generated, in total $n_{i,j}$ fragments.

As a corollary, a subgraph $MaxF(G)_{i,j}$ is indexed to *each vertex* $i = 1, 2, \ldots, n_{i,j}$ or:

$$k \in MaxF(G)_{i,j} \Leftrightarrow i \in MaxF(G)_{k,j} \tag{20}$$

which is obvious. Note that *CJF* and *SZF* criteria do not induce such degeneration of fragments, due to the path exclusion and/or the equidistant vertex exclusion.

In case of *CMaxF* fragmentation, the occurrence of subgraphs comes from that of *MaxF* fragmentation. In the above example:

$$CMaxF(G, x) = 2 \cdot 5 \cdot x^7 + 2 \cdot 6 \cdot x^6 + 10 \cdot 11 \cdot x^1 \tag{21}$$

It is not surprising, since, by definition, for each $MaxF(G)_{i,j}$ a subgraph $CMaxF(G)_{i,j}$ is generated.

Theorem 5 *For the fragments SZF, CJF, MaxF and CMaxF, the following relation is true:*

$$n_G \cdot n_G - 1 = \Sigma n_{MinF} \leq \Sigma n_{CMaxF} \leq \Sigma n_{CJF} \leq \Sigma n_{SZF} \leq \Sigma n_{MaxF} \\ \leq n_G \cdot (n_G - 1)^2$$

Demonstration: indeed, $n_G \cdot (n_G - 1) = \Sigma n_{MinF}$ based on *MinF* definition; $\Sigma n_{MinF} \leq \Sigma n_{CMaxF}$ is true because always $\{i\} \in V(CMaxF(G)_{i,j})$; $\Sigma n_{CJF} \leq \Sigma n_{SZFj}$ is true because *CJF* are generated by applying *SZ* criterion on G_p, where p is the path, joining i with j, to be deleted from G; $\Sigma n_{SZF} \leq \Sigma n_{MaxF}$ because $SZ(G)_{i,j}$ is a subgraph of $MaxF(G)_{i,j}$ (equation 18); $\Sigma n_{MaxF} \leq n_G \cdot (n_G - 1)^2$ is true because $n_G \cdot (n_G - 1)^2$ is the maximum possible value of Σn_{MaxF}. It results from: the maximum size of fragment $MaxF(G)_i, n_{MaxF} = n_G - 1$, and next, the number of all non-diagonal entries in the matrix is $n_G \cdot (n_G - 1)$, thus obtaining max $(\Sigma n_{MaxF}) = n_G \cdot (n_G - 1)^2$.

5 Conclusions

Subgraphs obtained by applying several fragmentation criteria have been investigated. Two new criteria have been defined and characterized along with the well known criteria Szeged and Cluj. The matrix and polynomial representations of vertices composing each type of subgraphs have been discussed. Analytical formulas for the polynomials of several classes of graphs have been derived. The newly introduced subgraphs/fragments, called *MaxF* and *CMaxF*, appeared to have interesting properties, which have been demonstrated.

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