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Original Scientific Paper

On Complexity of Transitive Graphs Representing Degenerate Rearrangements*

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Graphs representing degenerate rearrangements are vertex and edge transitive. First such graph of interest in chemistry was considered by Balaban. It describes the rearrangements of trigonal bipyramid complex XY_5 by a mechanism in which axial bonds become equatorial and three equatorial bonds become axial. We will discuss complexity of such graphs based on considering the shells of neighbors at increasing distance from a single vertex.

Key words: transitive graphs, degenerate rearrangements, complexity index, augmented valence, monster graphs.

INTRODUCTION

Graph theory is a branch of discrete mathematics concerned with relations between objects. In applications of graph theory to chemistry most often atoms are considered as vertices and chemical bonding as a relation. This results in representation of molecules by molecular graphs that display molecular connectivity.[1] Besides molecular graphs based on adjacency of atoms in a molecule there are other kinds of molecular graphs. For example Joela[2,3] introduced graphs based on considering relations between neighboring CC double bonds in Kekulé valence strustures. Several people considered various relationships between π-electron sextets in Kekulé valence structures, which resulted in the so called Gutman trees,[4] Clar graphs[5] and

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* Dedicated to Professor Smiljko Ašperger on the occasion of his 80th birthday.

the resonance graphs[6] in which only relationship between qualified Kekulé valence structures were considered.

There is yet another important class of chemical graphs which are concerned with representing chemical reactions.[7] The elements in such graphs are molecules entering reaction and product of reactions while the edges are the reaction routes. An important subgroup of reaction graphs are graphs depicting degenerate isomerizations. In this case the starting molecule and the resulting molecule of »chemical reactions« is the same chemical structure in which only the labels of atoms making bonds have changed. The simplest case represents the Cope rearrangement and the hypothetical »oscillations« or »resonance« between the two Kekulé valence structures of benzene, illustrated in Figure 1. Both cases are represented by a simple graph having two vertices connected by a single edge (line).

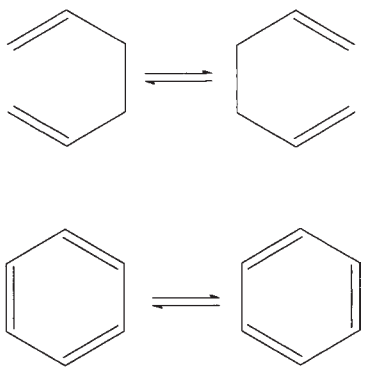


Figure 1. Cope rearrangment and Kekule valence structures of benzene.

Graph representing degenerate rearrangements were introduced into chemistry by Balaban in his pioneering paper about 35 years ago.[8] The first non-trivial graphs representing degenerate rearrangements are the Peterson graph (G_1) (Figure 2) and the Desargues Levi graph (G_2) of Figure 3. The Petersen graph depicts connections between ten isomers of trigonal bipyramid (AB)(CDE), where labeled atoms (all of the same kind) are grouped into axial and equatorial.[9] The Desargues-Levi graph depicts connections between twenty isomers of trigonal bipyramid in which we differentiate between enatiomers (AB)(CDE) and (AB)(EDC), which is its mirror image.[8,10] Levi, who was a mathematician, has shown that one can associate a graph with various mathematical configurations of lines and points. Thus the Desargues-Levi graph, which was the graph introduced in chemistry by Balaban, also depicts the Desargues configuration of geometry.

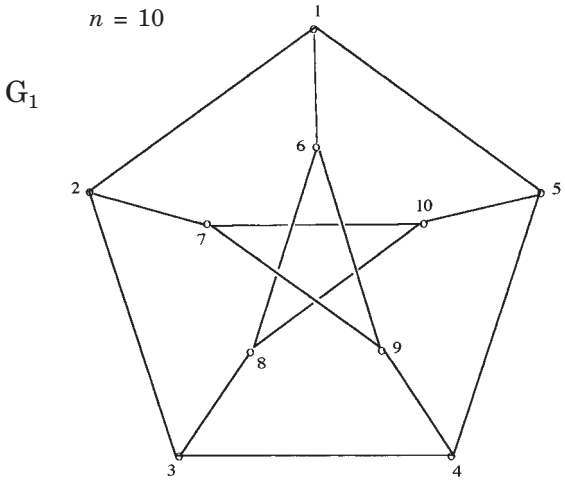


Figure 2. The Petersen graph (G_1).

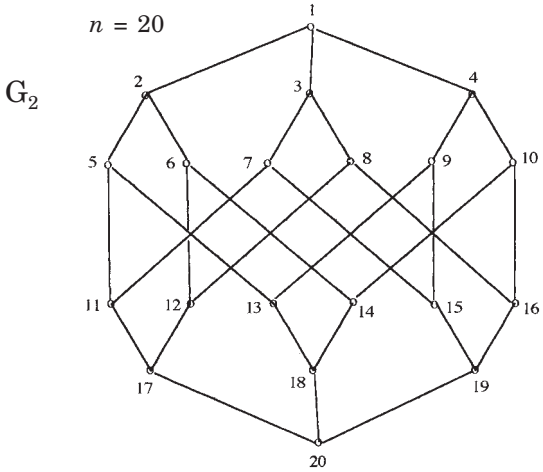


Figure 3. The Desargues-Levi graphs (G_2).

Graphs depicting degenerate rearrangements soon attracted attention of many chemists.[11] These »rearrangement graphs« are classified as vertex and edge transitive, which means that all vertices and all edges are mutually equivalent. They became a subject of numerous studies, several of which were focusing on the symmetry properties of these graphs.[12–14] To a non initiated person in graph theory the problem to determine the symmetry of graphs in general and transitive graphs in particular may appear if not trivial then a straightforward exercise in graph theory. In fact the prob-

lem is difficult and comparable to the problem of finding Hamiltonian circuit,[15] which is known to be NP,[16] that is, a problem which cannot be solved by a polynomial algorithm.[17]

In this paper we will focus attention on the complexity of graphs representing degenerate rearrangements. We have selected a dozen such graph from the literature and will consider their relative complexities.

ON COMPLEXITY OF GRAPHS

The topic of complexity of graphs received considerable attention in the chemical literature,[18–26] despite that the concept of the complexity of a mathematical object, graph included, is at best a qualitative. There is no clear and well defined concept of molecular complexity or graph complexity. Most people agree that complexity of a system increases as the number of components that constitute the system increase. In the case of molecular graph this means that complexity increases as the number of atoms in a molecule increases and as the number of bonds increases, both being associated with increase in the branching and cyclicity of a system. But again neither branching nor cyclicity are well defined structural concepts. It is also agreed that symmetry should also play a role in characterization of complexity of a system. In Table I we show several approaches to characterization of complexity, most of which proposed various complexity indices as a measure of complexity.

It is not uncommon in chemistry to come across useful notions which have generally well understood qualitative character but elude quantitative characterization. These, besides branching and cyclicity, include for example the notions of aromaticity and resonance energy, molecular surface and mo-

TABLE I

List of alternative complexity indices

Invariant	Method	Authors	Ref.
Neighborhood	information theory	Basak *et al.*	23
Paths	total number	Randić *et al.*	27
Wiener index		Bonchev & Trinajstić	19
Walks	total number	Rücker & Rücker	29
Spanning trees	total number	Trinajstić *et al.*	25
Partition	Shannon formula	Bertz	22

lecular volume, and of course, molecular shape. What is common to all such concept is »definition-less,« that is the lack of rigorous mathematical definition of such concept. A way out of this quagmire is to select a quantity, an index, to measure the »degree« of the quality considered. While this is not only legitimate but under the circumstances the only prudent procedure the approach itself may bring disagreements between different authors. The situation is very similar to that encountered when considering »the degree« of similarity between mathematical, geometrical, or graph theoretical objects. It need not be that one approach is better than another, but rather that different approaches focus attention on different aspects of similarity. Hence we should expect, in parallelism with the problem of quantifying the degree of similarity within a set of objects, that the determination of the complexity between systems considered can only be discussed relative to the descriptors used to characterize complexity. In other words, there is no an absolute complexity measure but only relative. Two molecules may be of similar complexity when characterized by the number of paths, and walks, but may not be similar when characterized by partition into bond types or in the case of benzenoid hydrocarbons when decomposed into Kekulé valence structures.

When considering similarity among molecules one can use as molecular descriptors paths of different length,[27] the count of walks or self-returning walks,[28,29] paths/walks quotients,[30] the leading eigenvalues of ${}^{m}\boldsymbol{D}/{}^{m}\boldsymbol{D}$ matrices,[31] and so on. In each case the resulting similarity among molecules reflects the similarity with respect to path, walks, self-returning walks, weighted walks, path/walks quotients, *etc*. So we believe that similarly we can speak of the complexity with respect to the number of paths,[27] the number of spanning trees,[25] the number of nearest neighbors,[23] the total number of walks,[29] the magnitude of augmented valence,[32] *etc*. We will in this contribution use the complexity index based on the concept of augmented valence illustrated in the following section of several smaller graphs.

AUGMENTED VALENCE AS A COMPLEXITY INDEX

The simplest vertex/edge transitive graphs are graphs C_n representing cycle having n vertices and n edges. Additional family of well known-vertex and edge transitive graphs are n-dimensional cubes. In Table II we have listed complexities for the above mentioned graphs based on the augmented valence, an index of complexity that we have adopted for study of transitive graphs of degenerate rearrangements reported in this paper. Similarly the complete bipartite graphs $K_{n,n}$ and the complete graphs K_n are also vertex/edge transitive. In Table III we have listed complexities for $K_{n,n}$ and K_n graphs based on the augmented valence.

TABLE II

List of neighbors at different distance and the complexity indices, C, for the family of graphs representing cycles on increasing size

	Family of graphs									
Cycles	0	1st	2nd	3rd	4th	5th	6th		C	C/V[a]
C_3	1	2						2	4	1.3333
C_4	1	2	1					2.25	4.5	1.1250
C_5	1	2	2					2.5	5	1.0000
C_6	1	2	2	1				2.625	5.25	0.8750
C_7	1	2	2	2				2.75	5.5	0.7857
C_8	1	2	2	2	2	1		2.8125	5.625	0.7031
C_9	1	2	2	2	2	2		2.8281	5.6562	0.6285
C_{10}	1	2	2	2	2	2	1	2.90625	5.81250	0.58125
C_{11}								2.93750	5.87500	0.53409
C_{12}								2.95313	5.90625	0.49219
C_{13}								2.96875	5.93750	0.45673
C_{14}								2.97656	5.95313	0.42522
C_{15}								2.98438	5.96875	0.39792
C_{16}								2.98828	5.97656	0.37354
C_{17}								2.99219	5.98438	0.35202
C_{18}								2.99414	5.98828	0.33268
C_{19}								2.99609	5.99219	0.31538
C_{20}								2.99707	5.99414	0.29971
C_∞								3.00000	6.00000	0.00000

[a] V, the number of vertices in a graph.

The index of augmented valence is obtained as follows: For each vertex in a graph we write the sequence of the valences of their neighbors at increasing separation. In case of vertex transitive graphs in which necessarily all vertices have the same vertex degree such sequence can be easily obtained from the list of neighbors at increasing distance. For example, in the case of a cube the list of neighbors at different distances is 1, 3, 3, 1, which if multiplied by three (the degree of vertices) gives for the list of neighbor valence: 3, 9, 9, 3. Augmented valence is obtained by taking successive valence of graph vertices with decreasing weights: 1, 1/2, $1/2^2$, $1/2^3$, *etc*. and adding all such contributions. Thus in the case of cube we obtain for a single vertex

TABLE III

List of neighbors at different distance and the complexity indices for the family of graphs representing n-dimensional cubes, complete bipartite graphs $K_{n,n}$ and complete graphs K_n

	Family of graphs									
n-cubes	0	1st	2nd	3rd	4th	5th	6th	N	C[a]	C/V
1-cube	1	1						1.5	1.5	0.7500
2-cube	1	2	1					2.25	4.5	1.1250
3-cube	1	3	3	1				3.375	10.125	1.2656
4-cube	1	4	6	4	1			5.0625	20.25	1.2656
5-cube	1	5	10	10	5	1		7.5938	37.9688	2.3730
6-cube	1	6	15	20	15	6	1	11.3906	68.3438	1.0679
7-cube	1	7	21	35	35	7	...	17.0859	119.602	0.9344
8-cube	1	8	28	56	70	56	...	25.6289	205.031	0.8009
9-cube	1	9	36	64	126	126	...	35.7715	321.943	0.6288
$K_{n,n}$										
$K_{1,1}$	1	1						1.5	1.5	0.75
$K_{2,2}$	1	2	1					2.25	4.5	1.125
$K_{3,3}$	1	3	2					3	9	1.5
$K_{4,4}$	1	4	3					3.75	15	1.875
$K_{5,5}$	1	5	4					4.8333	24.1667	2.4167
$K_{6,6}$	1	6	5					5.25	31.5	2.625
$K_{7,7}$	1	7	6					6	42	3
$K_{8,8}$	1	8	7					6.75	54	3.375
$K_{9,9}$	1	9	8					7.5	67.5	3.75
K_n										
K_2	1	1						1.5	1.5	1.0000
K_3	1	2						2	4	1.3333
K_4	1	3						2.5	7.5	1.8750
K_5	1	4						3	12	2.4000
K_6	1	5						3. 5	17.5	2.9167
K_7	1	6						4	24	3.4286
K_8	1	7						4.5	31.5	3.9375
K_9	1	8						5	40	4.4444
....										

[a] $C = N \times d$.

augmented valence: 3 (1 + 3/2 + 3/4 + 1/8) = 10.125. This figure is an index of complexity in the case of transitive graphs, because there all vertices are symmetry equivalent, and are not contributing to the diversity. Observe that because all vertices in vertex transitive graphs are symmetry equivalent the local complexity index that refers to a single atoms is proportional to global (molecular) complexity index.

In Table II and Table III we show the list of neighbors at increasing distance and the derived complexity indices for a selection of well-known graphs: the C_n cycles, the n-dimensional cubes, the complete bipartite graphs and complete graphs. As we see from Table II and Table III the pattern of neighbors at different distances are very regular for these graphs. In the case of n-cubes the number of neighbors is given by binomial coefficients (that appear in the Pascal triangle). The quotient $C(x)/V$, where V is the number of vertices in a graph, gives an alternative measure for complexity.

The complexity indices of C_n, Q_n, $K_{n,n}$ and K_n can serve as the standards for comparison of the complexities of transitive graphs of degenerate rearrangements reported in this paper. In Figure 4 we plotted the complexity index C as a function of n, the graph index, for C_n. From the figure we see that the complexity C-index for cycles shows convergence as n, the size of cycles, increaes indefinitely. It is easy to show that C-index converges to 6, given by the limit of the series 2 x [1 + 2 (1 + 1/2 + 1/4 + 1/8 + 1/16 + 1/32 + 1/64 + 1/128 +...)]. In Figure 5 we compare the increase of C-index for the n-cubes, the complete bipartite graphs $K_{n,n}$ and the complete graphs K_n with the in-

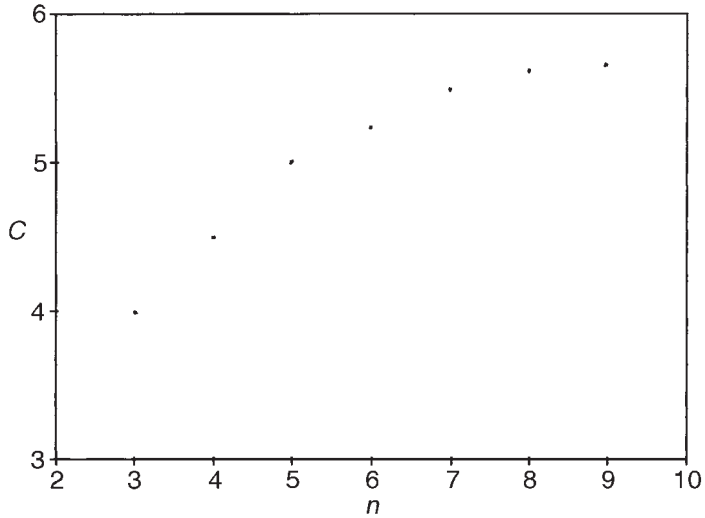


Figure 4. Convergence of the complexity index for cycles as n increases.

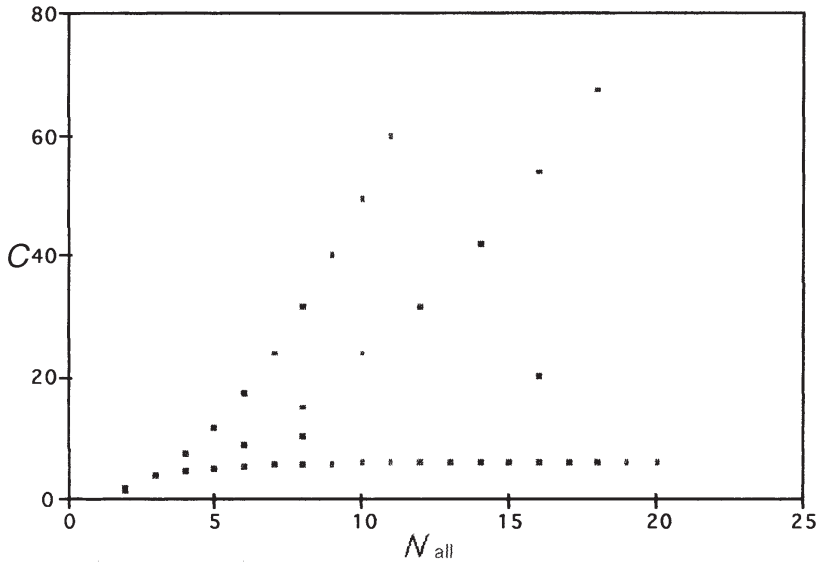


Figure 5. Variation of the complexity index of the complete graph K_n, complete bipartite graph $K_{n,n}$, and the n-dimensional cubes with increase in number of vertices.

TABLE IV

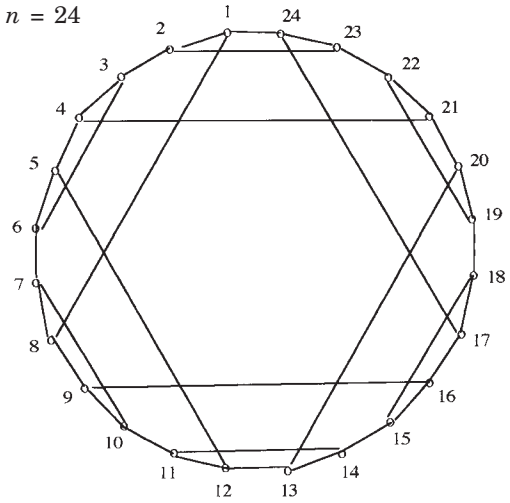
List of neighbors at different distance and local and global complexity indices for mathematical graphs of Figure 5 and Figure 6

	Graphs							Complexity		Smallest ring
	0	1st	2nd	3rd	4th	5th	6th	Local	Global	
Figure 5										
G_3 n = 24	1	3	5	6	5	3	1	14.76563	354.375	4
G_4 n = 24	1	3	6	7	7	1		16.03125	384.75	4
G_5 n = 24	1	3	6	9	5			16.3125	391.50	6
G_6 n = 24	1	3	6	11	3			16.6875	400.50	6
Figure 6										
G_7 n = 14	1	3	6	4				13.5	189	
G_8 n = 16	1	3	5	6	1			14.0625	225	
G_9 n = 18	1	3	6	6	2			14.625	263.25	
G_{10} n = 18	1	3	6	6	2			14.625	263.25	
G_{11} n = 18	1	3	6	6	2			14.625	263.25	
G_{12} n = 30	1	3	6	12	8			18	540	

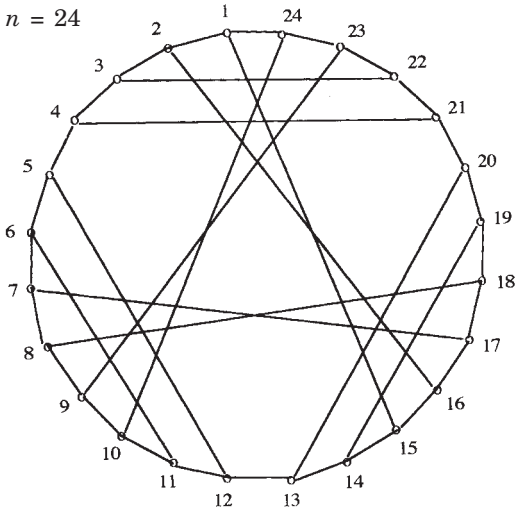
crease in size of these graphs measured by V, the number of vertices. As expected for graphs having the same number of vertices the complete graphs are the most complex, then come the complete bipartite graphs and then n-cubes.

In Table IV we consider several vertex transitive graphs from the mathematical literature shown in Figure 6 and Figure 7.[33,34] Graphs G_3–G_6 of Figure 6 have 24 vertices and have been constructed using 4×4 permutation matrices as generators.[33] Graphs of Figure 7 include the Heawood graph

G_3



G_4



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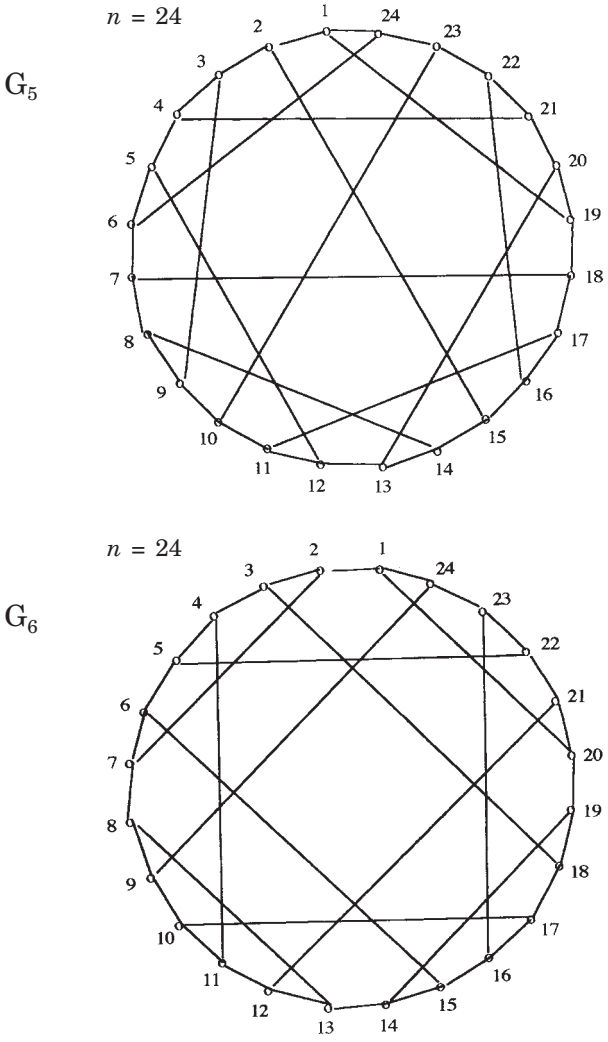


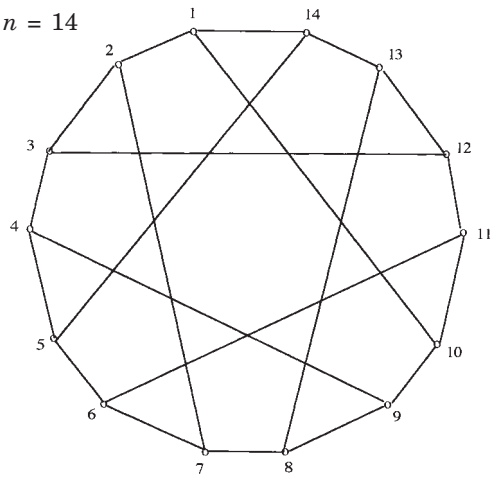
Figure 6. Four transitive graphs (G_3–G_6) generated by 4=4 permutation matrices having 24 vertices.

(G_7) having n = 14 vertices, which is also the Levi graph of the Fano configuration, the Möbius-Kantor graph (G_8) having n = 16 vertices, the Levi graph of three 9_3 configurations (G_9–G_{11}) having n = 18 vertices, G_{11} being the graph of the Pappus configuration), and the Levi graph of the Cremona--Richmond configuration (G_{12}) having n = 30 vertices. We can see from the upper part of Table IV which gives the complexities for the four trivalent (cubic) graphs having n = 24 vertices vary considerably even though all

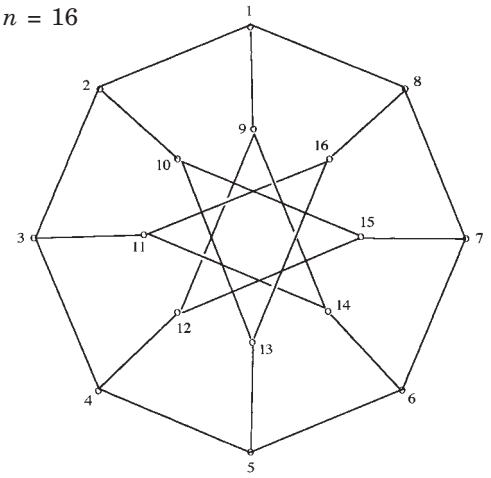
graphs are of the same size. It appears that the index of complexity increases as the size of the smallest rings in such graph increase.

The list of neighbors already gives some insight into the complexity of graphs. As we see from Table IV the number of second neighbors is the smallest for G_3 and graphs G_4–G_6 which have the same number of second neighbors are ordered according the number of third neighbors. The length of list of neighbors immediately gives the diameter of a graph, however one can also obtain from the list information on smallest ring size. One can deduce the site of »ring closure,« which is determined by the place in the sequence when the next member in a sequence is not of the form $(v - 1)^k$,

G_7 $n = 14$



G_8 $n = 16$



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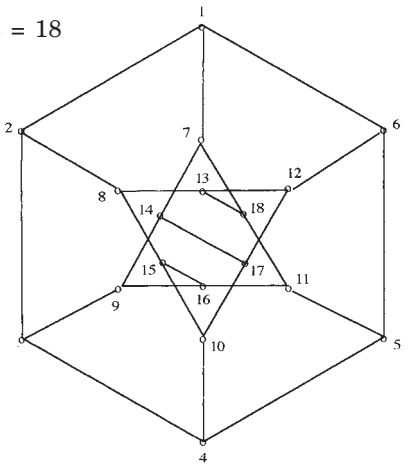
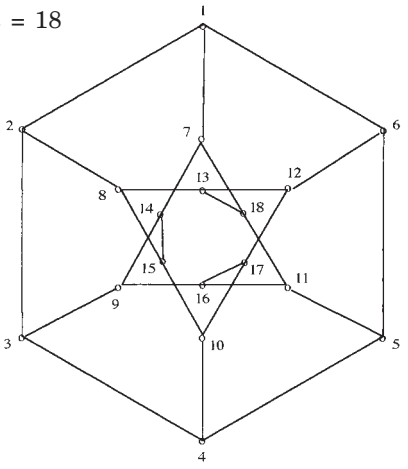
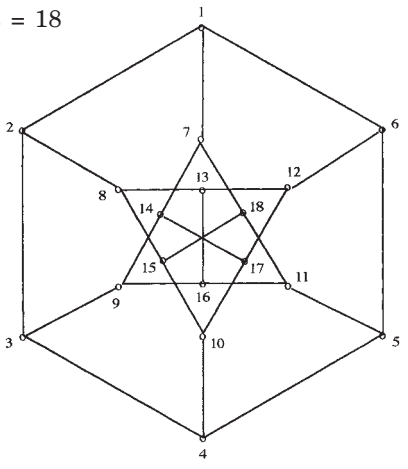
G_9 $n = 18$



G_{10} $n = 18$



G_{11} $n = 18$



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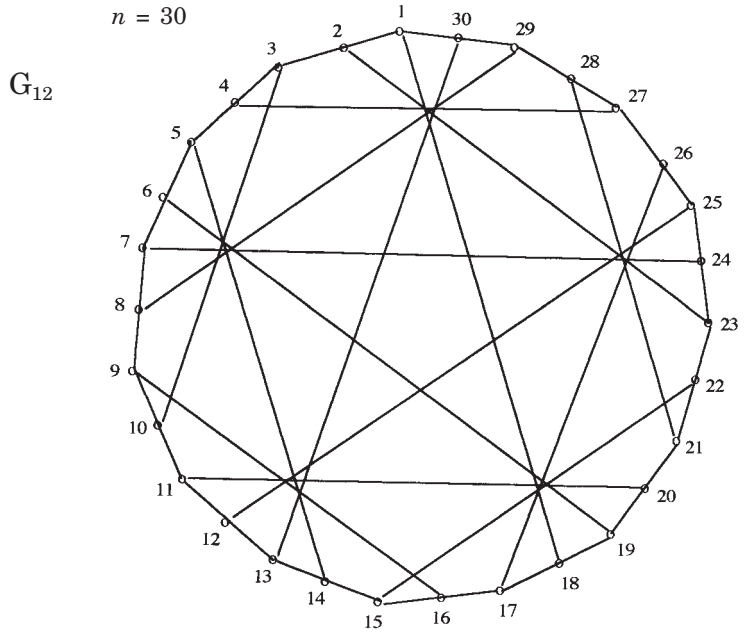

Figure 7. A selection of vertex transitive graphs from mathematical literature. G_7: the Heawood graph (which is the Levi graph of the Fano configuration); G_8: the Möbius-Kantor graph; G_9–G_{11}: the Levi graph of three 9_3 configurations, (G_9 is the Levi graph of Pappus configuration); and G_{12}: the Levi graph of the Cremona-Richmond configuration.

where v is the degree of vertex and k is the distance of the neighbor from that vertex (excluding the first two members of the sequence which are always 1, v). In the case of trivalent graphs one should compare neighbor sequence with the sequence 1, 3, 6, 12, 24, 48, 96,... which would be the sequence of neighbor in Bethe lattice (an infinite acyclic structure in which every vertex has three neighbors).

Comparison of complexity of graphs of different size and different valence is less straightforward. Apparently the size of a graph dominates the complexity index when valence of graphs are the same. As we see from Table V non-isomorphic graphs can have identical lists of neighbors (and the same valence) as is the case with graphs G_9–G_{11} representing different 9_3 configurations of geometry. Hence, necessarily such graphs will have the same complexity. The three graphs when superimposed one on another show that they differ only in connectivities of the central six vertices 13–18. Interestingly the six central vertices have patterns of adjacency which we find in Dewar, Kekulé and Claus formulas of π-electrons of benzene.

TRANSITIVE GRAPHS OF DEGENERATE ISOMERIZATIONS

The Petersen graph (G_1) and the Desargues-Levi graph (G_2) are associated with neighbor sequences 1, 3, 6 and 1, 3, 6, 6, 3, 1, respectively. The corresponding complexities are 3 (1 + 3/2 + 6/4) and 3 (1 + 3/2 + 6/4 + 6/8 + 3/16 + 1/32) which give respectively 12.00000 and 14.90625. The complexity index here considered shows non linear dependence on size of a system and reflects the fact that more distant vertices make lesser contributions to local complexity of a vertex. In this respect augmented valence is an index of local environments of an atom. The distinction between the Petersen and the Desargues-Levi graph, if we confine interest to the nearest and the next nearest neighbor, *i.e.*, the sequence 1, 3, 6, is that in the Petersen graph the next nearest neighbors are connected among themselves resulting in ring closures, while this is not the case with the Desargues-Levi graph.

In Table V we give list of neighbors and computed complexities for graphs G_{13}–G_{18} representing different degenerate rearrangements. Graphs are illustrated in Figures 8–11. Graph G_{13} represents an intramolecular rearrangement of tetragonal-pyramidal complex,[35] while graphs G_{14} and G_{15} illustrate intramolecular isomerization of trigonal bi-pyramidal structures with five different ligands.[36] Graphs G_{16} and G_{17} illustrate intramolecular

TABLE V

List of neighbors at different distance and local and global complexity indices for chemical graphs of Figure 8 to Figure 11

	Graphs					Complexity	
	0	1st	2nd	3rd	4th	Local	Global
Figure 8							
G_{13} $n = 15$	1	4	8	2		5.125	76.875
Figure 9							
G_{14} $n = 10$	1	6	3			28.5	285
G_{15} $n = 20$	1	6	9	4		40.5	810
Figure 10							
G_{16} $n = 15$	1	6	8			36	540
G_{17} $n = 15$	1	8	6			46	690
Figure 11							
G_{18} $n = 30$	1	4	10	14	1	29.25	877.50

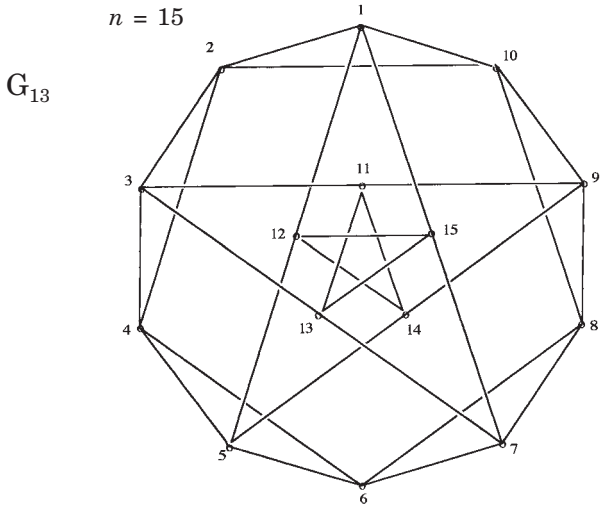

Figure 8. Pictorial representation of graph of an degenerate rearrangement of tetragonal pyramidal complexes (from Ref. 35).

isomerization of octahedral complexes with six different ligands,[37] and the graph G_{18} with $n = 30$ vertices is a reaction graph for degenerate rearrangements of homovalenium cations.[38] Of particular interest is to compare graphs of the same size or of the same valence visually and then see if the numerical characterization reflects expectations. Such comparison shows that the local complexity index is very sensitive to the valence rather than size if the two are different. Thus, for example graph G_7 with $n = 30$ is barely more »complex« than the graph on only ten vertices (G_{14}) but vertices having larger valence. The global complexity index will be sensitive to the size of a graph which for transitive graphs is obtained by multiplying the local complexity with V, the number of vertices. In the last column in Table IV and Table V we have listed these global complexity values. Again we find that smaller graphs having larger valence may have comparable overall complexity to larger graphs having smaller valence. This is illustrated by graphs G_{15} and G_{18}.

MONSTER GRAPHS

Graphs having unusually large number of vertices have been referred to as »monster« graphs. Two such graphs have appeared in chemical literature. The first graph represents degenerate rearrangements of P_7^{3-} studied experimentally by Baudler and coworker.[39] This »baby« monster graph of degenerate rearrangements of P_7^{3-} has 7!/3 or 1680 vertices. The graph was

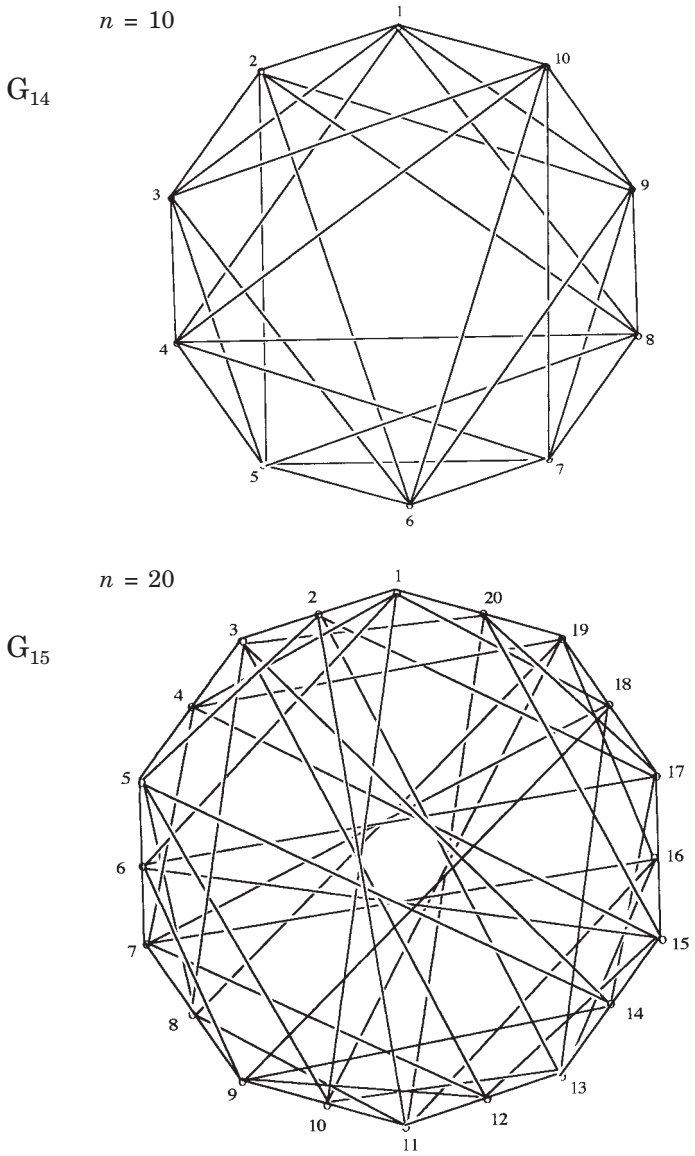

Figure 9. Topological representation of rearrangement modes $M_4(6)$ (top) and $M_2(6)$ (bottom) of intramolecular isomerizations of trigonal bipyramidal structures as depicted by A. T. Balaban (Ref. 36).

studied by Randić, Oakland and Klein[13] who reported the list of neighbors at different shells of distance to be:

1, 3, 6, 12, 24, 45, 81, 147, 255, 365, 350, 231, 116, 37, 7.

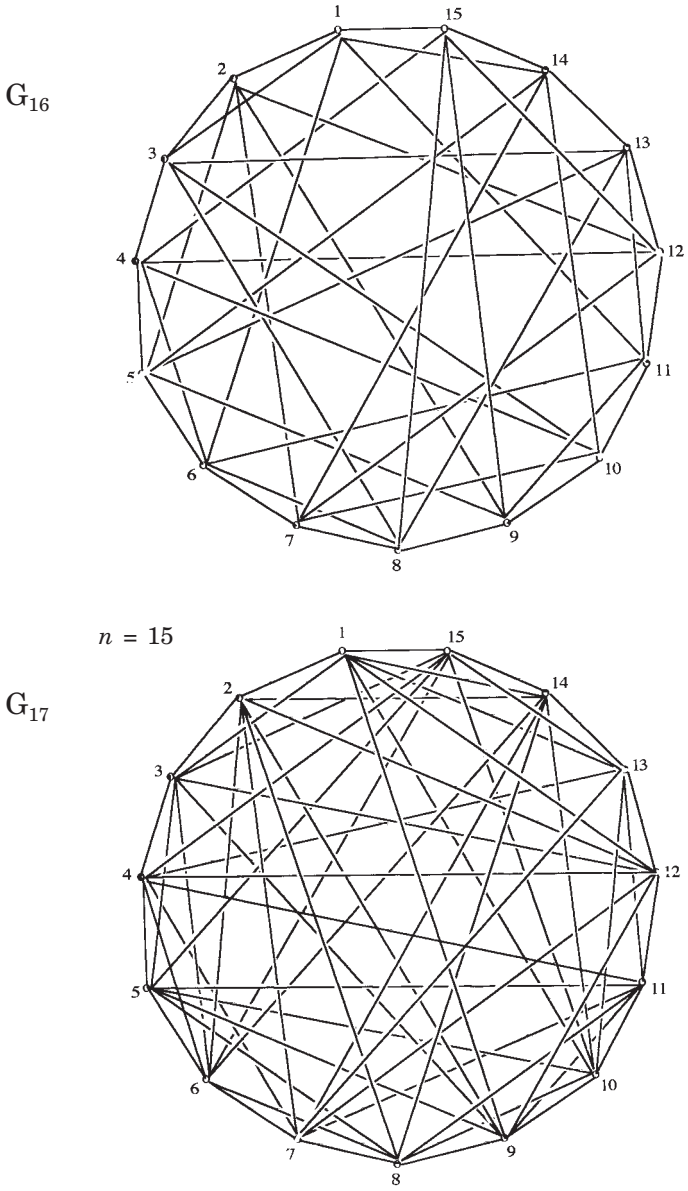

Figure 10. Graph representing isomerization of octahedral complexes *via* diagonal twist and the rhombic twist mode (as depicted by A. T. Balaban in Ref. 37).

In total there are 15 shells counting also the starting (central) vertex. From this list of neighbor at different distance the complexity index follows to be: 38.0260620117. At the first glance this may appear as not so large

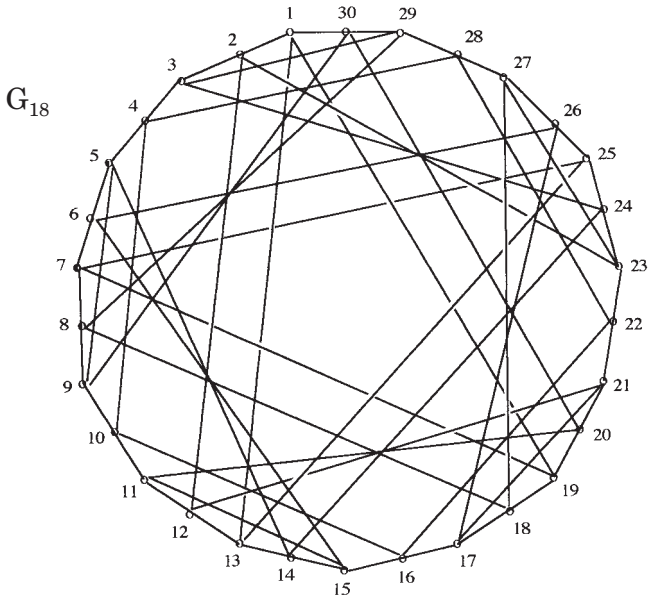

Figure 11. Rearrangment graph for homotetrahedral cation $C_5H_5^+$ (Ref. 38).

value, the graph having lesser local complexity then graphs G_{15} (Figure 9) and graph G_{17} (Figure 10), however, one should keep in mind that the »baby« monster graph is a cubic graph, and hence, its complexity should be compared to cubic graphs, such as graphs of Table IV, where the most complex is the graph having $n = 30$ vertices whose complexity index is only 18. If one is to consider global complexity by adding all local contributions then for »baby« monster we would obtain: 63 883.78 which is larger by two orders of magnitude than the most complex graph of Table V.

The second »monster« graph represents degenerate rearrangement of bullvalene $C_{10}H_{10}$ conceived by Doering[40] and synthesized by Schröder and coworkers.[41] The graph has 10!/3 or 1 209 600 vertices. The list of neighbors at different distances for the »monster graph« was reported by Živković:[42] 1, 3, 6, 12, 24, 48, 93, 177, 339, 651, 1242, 2327, 4341, 8040, 14682, 26343, 46446, 79021, 126085, 183648, 231697, 232096, 163373, 70564, 16343, 1848, 125, 21, 3, 1.

In total there are 30 shells of neighbors counting also the starting (central) vertex. From this it follows that the local complexity index is: 67.6348287631. When this number is multiplied by the number of vertices we obtain 81 811 088.8718, a number which is larger than the global complexity of the »baby« monster by three orders of magnitude. This in itself justifies referring to the smaller monster graph as a »baby« monster.

DISCUSSION

We have to emphasize that graph that may have identical or close complexity indices based on the augmented valence may differ more when some other measure of complexity is considered. We will not pursue this interesting aspect of complexity here, except to mention that this suggests that, at least for now, instead of a single absolute index of complexity there may be several alternative characterizations of complexity. However, in addition to *ad hoc* collection of diverse complexity indices, one could consider possibility of having mathematically related complexity indices that can be viewed as the »higher order« complexity indices.

The situation in assigning to a graph complexity index is to some extent similar to attributing to a graph a branching index.[43] As is known several branching indices have been proposed in chemical and mathematical literature, starting with the suggestion by Lovasz and Pelikan[44] that the leading eigenvalue of the adjacency matrix may serve as such. It happens that 2,2-dimethylhexane and 2,5-dimethylhexane, both have identical leading eigenvalue, hence according to Lovasz and Pelikan, the two octane isomers which certainly look distinctive have the same »branching« degree. Other branching indices have different pairs of graph showing similar degeneracy. These cases of coincidence, when two or more non isomorphic graphs show degeneracy for selected topological indices, should be of considerable interest as they can help in clarifying interpretation of such indices. For instance, since branching parallels complexity, and in numerous instances graphs of apparently different branching have the same leading eigenvalue it is clear that the leading eigenvalue is at best an index of branching of limited potential. However, the leading eigenvalue may well be an index of some other structural characteristics of molecular graphs with parallel branching to some extent – including being an index of molecular complexity! There is nothing intrinsic to the concept of complexity that would not allow that molecules of apparently different branching (like 2,2-dimethylhexane and 2,5-dimethylhexane) may not have the same complexity.

CONCLUDING REMARKS

Transitive graphs offer useful representation of complex degenerate chemical transformations. Hitherto only few properties of such graphs, have been considered. This, includes construction of generating permutation matrices, determination of symmetry of such graphs, and in the case of monster graphs finding the size of the smallest cycle and finding the number of neighbors at different distance. That determination of the number of nearest neighbors at different distances is quite involved can be seen from published reports, but even to determine the size of the smallest cycle in such graphs in itself

is not so simple. This is reflected, for instance by an incorrect report for the smallest cycle in bullvalene graph to be of size 14,[45] when in fact it is of size 12 (see Ref. 13). Determination of the symmetry properties of graphs in general, and transitive graphs in particular, is another seemingly straightforward but in fact very complex problem.[16,17]

In this contribution we derived an alternative numerical characterization of transitive graphs, referred to as complexity index. The new index is based on simple manipulations of valences of neighbors at different distance from a vertex considered. The valences of distant neighbors are combined in a single »augmented valence,« the quantity taken as a measure of complexity. In view that transitive graphs are regular (*i.e.*, all vertices are of the same degree) already the list of neighbor at different separation from the vertex considered offers qualitative indication of complexity of such graphs, but when combined with appropriate weights produce a single graph invariant that we have taken as a measure of complexity of such graph. In doing this we have avoided the difficult problem of trying to define complexity in more rigorous mathematical fashion – the task that awaits to be considered.

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SAŽETAK

O složenosti tranzitivnih grafova koji predstavljaju degenerirane pregradnje

Milan Randić

Grafovi koji predstavljaju degenerirane pregradnje jesu čvorno i bridno tranzitivni. Prvi takav graf od kemijskog interesa razmatrao je Balaban. Taj graf opisuje pregradnju trigonskog bipiramidnog kompleksa XY_5 mehanizmom u kojemu aksijalne veze postaju ekvatorijalne, a dvije ekvatorijalne veze aksijalne. Razmatrana je složenost tranzitivnih grafova koji predstavljaju degenerirane pregradnje, i to s pomoću ljusaka susjeda kojima se udaljenost od pojedinog čvora povećava.