

On the Zagreb Indices as Complexity Indices[#]

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Two original Zagreb indices, denoted M_1 and M_2 , and introduced in 1972, were symmetry-modified by summing up only degrees (SMM_1) or edge-weights (SMM_2) of symmetry nonequivalent vertices or edges of graphs. Their dependence on the structural features and symmetry of molecular graphs is studied. They were also compared to eight other complexity indices (RCI , TC , $TC1$, BT , BI , twc , wcx) on nine graphs (A, B, C, D, E, F, G, H, I) with five vertices that were earlier studied by several research groups. The TC , $TC1$ and N_t produce exactly the same complexity ordering of nine graphs ($I > H > G > F > E > D > C > B > A$). The ordering produced by M_1 is different from this ordering in that it cannot discriminate E and F, and C and D. Likewise, M_2 and twc produce exactly the same ordering and the latter ordering differs from the former only in the reverse order of E and F. Orderings produced by SMM_1 and SMM_2 differ considerably from orderings given by TC , $TC1$ and N_t or M_2 and twc .

Key words: complexity indices, molecular graphs, saturated hydrocarbons, Zagreb indices.

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In this note we discuss the use of the so-called Zagreb indices¹⁻⁴ and their novel variants as complexity indices. The research we report was stimulated by the paper of Bertz and Wright⁴ in which they pointed out that the Zagreb M_1 index has the characteristics of a complexity index.

In the early work of the Zagreb Mathematical Chemistry Group on the topological basis of the π -electron energy, two terms appeared in the approximate formula for the total π -energy of conjugated molecules,^{5,6} which were later used separately as topological indices in QSPR/QSAR studies.^{2,3,7-9}

The original Zagreb indices (also referred to as the Zagreb Group parameters) are defined as follows:

$$M_1 = \sum_i d(i)^2 \quad (1)$$

$$M_2 = \sum_{\text{edges}} d(i)d(j) \quad (2)$$

where $d(i)$ is the degree of the vertex i and $d(i)d(j)$ is the weight of the edge $i-j$.

Since many authors who derive and use molecular complexity indices employ concepts and terminology of (chemical) graph theory^{10,11} in their work, we do the same. Graphs are generated from molecules by replacing atoms with vertices and bonds with edges. We consider only saturated hydrocarbons and the corresponding graphs depicting their carbon skeletons.

The M_1 index can be also computed by means of the line graph^{10,11} of a graph.¹² The M_1 index of a graph G equals twice the number of vertices and edges of a corresponding line graph L :

$$M_1 = 2 [V(L) + E(L)] \quad (3)$$

where V is the number of vertices and E is the number of edges in L . Bonchev¹³ found that the M_1 index is also related to the number of self-returning walks¹⁴ of four steps (4SRW):

$$M_1 = ({}^4SRW + 2 E)/2. \quad (4)$$

The consequence of this relationship is the following result: The M_1 index produces exactly the same ordering of isomeric molecules as the one produced by 4SRW .

The M_1 and M_2 indices can be given in a closed form for homologous structures. Here we give analytical formulas for n -alkanes and cycloalkanes:

(i) n -alkanes

$$M_1 = 4(n - 2) + 2 \quad (5)$$

$$M_2 = 4(n - 2) \text{ for } n > 2 \quad (6)$$

(ii) cycloalkanes:

$$M_1 = M_2 = 4n \quad (7)$$

where n is the number of vertices in a cycloalkane.

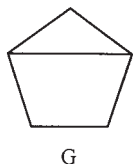
Most authors agree that the complexity of saturated hydrocarbons increases with increasing size, increasing branching¹⁵ (of acyclics) and cyclicity¹⁶ (of cycle-containing graphs) and with decreasing symmetry. However, the relationship between complexity and symmetry is not quite simple. There are reports in the literature, even philosophical,¹⁷ pointing out that complexity and symmetry are two parallel characteristics of a molecular structure with only a slight influence on each other.

We first studied the dependence of the Zagreb indices M_1 and M_2 on structural features in a hierarchical order (size, branching, cyclicity) and symmetry of molecular graphs representing selected hydrocarbons. The results can be summarized as follows: (i) Zagreb indices increase with size, that is, M_1 and M_2 indices increase with increasing number of vertices and edges. In the case of n -alkanes and cycloalkanes, this is directly seen from formulas (4) and (5); (ii) Zagreb indices increase with branching, that is, M_1 and M_2 indices increase with the appearance of vertices of degree three or higher. For example, the values of M_1 and M_2 indices for n -hexane ($M_1 = 18$, $M_2 = 16$) are smaller than those for 3-methylpentane ($M_1 = 20$, $M_2 = 19$); (iii) Zagreb indices increase with cyclicity, that is, M_1 and M_2 indices increase with increasing number of cycles, since more and more vertices of degree three (or higher) appear in bi-, tri-,..., cycles. For example, the values of M_1 and M_2 indices for cyclohexane ($M_1 = M_2 = 24$) are smaller than those for bicyclo [2.2.0]hexane ($M_1 = 34$, $M_2 = 41$); (iv) Zagreb indices are not directly affected by symmetry. A good example to illustrate this point is comparison between 3,6,9-trimethylundecane ($M_1 = 56$; $M_2 = 57$) and 3,6,8-trimethylundecane ($M_1 = 56$; $M_2 = 57$). This result has prompted us to devise symmetry-modified M_1 and M_2 indices.

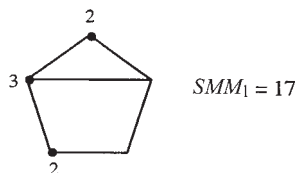
We symmetry-modified M_1 and M_2 indices by summing up only the degrees (edge-weights) of the symmetry nonequivalent vertices (edges). In doing this, we followed a recent suggestion by Randić¹⁸ and Rucker and Rucker.¹⁹ Of course, there are other possibilities open for the symmetry-adjustment of complexity indices, *e.g.* Ref. 20.

We denote symmetry-modified M_1 and M_2 indices by SMM_1 and SMM_2 . Computation of SMM_1 and SMM_2 indices is illustrated in Figure 1.

(i) Graph G depicting the carbon skeleton of bicyclo[2.1.0]pentane



(ii) Symmetry nonequivalent vertices denoted by black dots, their degrees and the SMM_1 index



(iii) Symmetry nonequivalent edges denoted by thicker lines, their weights and the SMM_2 index

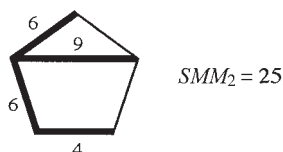


Figure 1. Computation of the symmetry-modified Zagreb SMM_1 and SMM_2 complexity indices for the bicyclo[2.1.0]pentane graph.

The SMM_1 and SMM_2 indices are closely related to the parent M_1 and M_2 indices for n -alkanes:

$$SMM_1 = \begin{cases} M_1/2 & n = \text{even} \\ (M_1/2) + 2 & n = \text{odd} \end{cases} \quad (8)$$

$$SMM_2 = \begin{cases} (M_2/2) + 2 & n = \text{even} \\ M_2/2 & n = \text{odd}. \end{cases} \quad (9)$$

It may be noted that $SMM_1(n\text{-alkane}) = SMM_1(n+1\text{-alkane})$ for $n = \text{odd}$ and $n \geq 3$ and $SMM_2(n\text{-alkane}) = SMM_2(n+1\text{-alkane})$ for $n = \text{even}$ and $n \geq 4$.

We also studied the dependence of SMM_1 and SMM_2 indices on the structural features of saturated hydrocarbons. The following results were obtained: (i) The SMM_1 and SMM_2 indices increase with size in groups of two in the case of n -alkanes, as can be seen from the above formulas. For cycloalkanes, the SMM_1 and SMM_2 indices are the same for any member of the series and are equal to four. This limits their usefulness as complexity indices for this class of structures; (ii) The symmetry-modified Zagreb indices are sensitive to branching, but show no trends: They may increase or decrease with branching. For example, 2-methylpentane has higher values of the SMM_1 and SMM_2 indices (19, 15) than n -hexane (9, 10) and more branched 2,3-dimethylbutane (10, 12); (iii) The symmetry-modified Zagreb indices increase with cyclicity. In comparing cyclohexane and bicyclo[2.2.1]hexane, one sees that the SMM_1 and SMM_2 indices are larger for bicyclic structures ($SMM_1 = 13$, $SMM_2 = 19$) than for similar monocyclic structures ($SMM_1 = SMM_2 = 4$). However, comparison between the members in the series bicyclo[2.2.0]hexane, tricyclo[2.2.0.0]octane, tetracyclo[2.2.0.0.0]decane, pentacyclo[2.2.0.0.0.0]dodecane, etc., shows that again the SMM_1 and SMM_2 indices increase with size in groups of two. Thus, $SMM_1 = 13$ and $SMM_2 = 19$ for both bicyclo[2.2.0]hexane and tricyclo[2.2.0.0]octane and $SMM_1 = 22$ and $SMM_2 = 37$ for both tetracyclo[2.2.0.0.0]decane and pentacyclo[2.2.0.0.0.0]octane; (iv) The values of symmetry-modified indices decrease with increasing symmetry of the system. This is so because the number of symmetry non-equivalent vertices and edges decrease with increasing symmetry. For example, the SMM_1 and SMM_2 indices for 3-methylpentane (15, 11) are smaller than these indices for less symmetric 2-methylpentane (17, 15).

A question that immediately arises is whether symmetry should dominate all other structural features of a molecule in designating complexity indices. There is disagreement between authors concerning this question. Some (e.g., Bertz^{4,21,22}) think that structural features should dominate symmetry, but symmetry must be included in the definition of the complexity index. Others (e.g., Randić¹⁸) support the view that in designing an index of molecular complexity, symmetry should have an important contribution. Some (e.g., Mainzer¹⁷) think that structural features and symmetry influence each other only to a certain degree. Finally, there is a fourth group (e.g., Bonchev,²³ Bertz and Sommer²⁴) who design complexity indices free of the direct influence of symmetry. Our standpoint is that the complexity index should depend on symmetry, but symmetry should not dominate other structural features of a molecule.

To compare the original and symmetry-modified Zagreb complexity indices with other complexity indices that were recently proposed, we use the set of nine graphs with five vertices that were studied first by Bonchev²³

and then by Randić¹⁸ and Rucker and Rucker.¹⁹ These graphs are shown in Figure 2 and a variety of their complexity indices is reported in Table I.

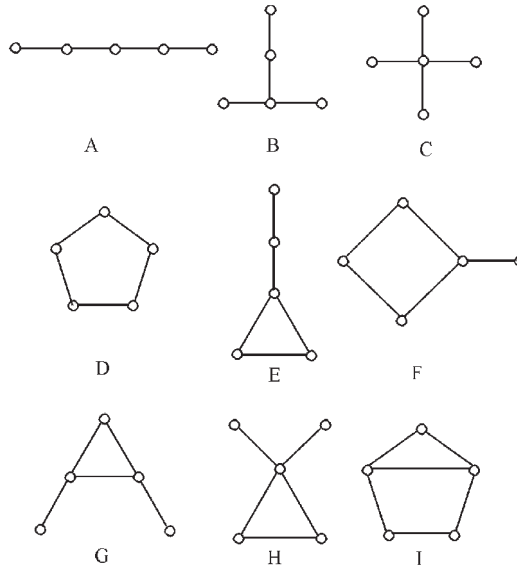


Figure 2. Nine simple graphs with five vertices.

TABLE I

Nine simple graphs from Figure 2 and some of their complexity indices

Graph label*	Complexity index [#]											
	M_1	M_2	SMM_1	SMM_2	RCI	TC	TCI	BT	BI	N_t	twc	wcx
A	14	12	9	6	11.4	60	40	18.47	7.51	15	44	28.0
B	16	14	15	11	16.1	76	50	15.22	14.00	17	53	44.0
C	20	16	17	4	9.8	100	64	9.71	15.51	20	70	32.5
D	20	20	4	4	5.0	160	110	10.00	11.61	26	75	15.0
E	22	24	18	18	19.6	172	112	14.86	27.02	27	93	71.5
F	22	23	18	13	19.9	190	126	13.61	27.02	29	89	69.5
G	24	27	14	18	15.6	212	136	13.61	33.30	31	107	66.0
H	26	28	21	16	16.8	230	146	10.00	42.00	33	116	74.5
I	30	37	17	25	18.8	482	310	9.71	49.06	54	150	89.5

* Labels correspond to graphs in Figure 2

[#] M_1, M_2 = original Zagreb indices;^{5,6} SMM_1, SMM_2 = symmetry-modified Zagreb indices; RCI = Randić complexity index;¹⁸ TC, TCI = Bonchev complexity indices;²³ BT = Bonchev-Trinajstić index;²⁵ BI = Bertz index;^{4,21,22} N_t = total number of connected subgraphs;^{23,24} twc = total walk count;¹⁹ wcx = walk complexity¹⁹

In Table I we report the following complexity indices: the original (M_1 , M_2) and symmetry-modified (SMM_1 , SMM_2) Zagreb complexity indices, the Randić complexity index (RCI),¹⁸ the Bonchev topological indices (TC , $TC1$),²³ the Bonchev-Trinajstić index based on graph-theoretical distances (BT),²⁵ the Bertz index (BI),^{4,21,22} the total number of connected subgraphs,^{23,24} the total walk count (twc),¹⁹ and the symmetry-modified twc called the walk complexity (wcx).¹⁹ The values of indices reported in Table I have been either computed by us or when available taken from the literature. In Table II we list the ordering of graphs from Figure 2 given by each complexity index from Table I.

TABLE II

Ordering of graphs from Figure 2 by complexity indices from Table I. Asterisks denote symmetry-independent indices.

Complexity index	Complexity ordering from the most to the least complex graph																
$*M_1$	I	>	H	>	G	>	F	=	E	>	D	=	C	>	B	>	A
$*M_2$	I	>	H	>	G	>	E	>	F	>	D	>	C	>	B	>	A
SMM_1	H	>	F	=	E	>	I	=	C	>	B	>	G	>	A	>	D
SMM_2	I	>	G	=	E	>	H	>	F	>	B	>	A	>	D	=	C
RCI	F	>	E	>	I	>	H	>	B	>	G	>	A	>	C	>	D
$*TC$	I	>	H	>	G	>	F	>	E	>	D	>	C	>	B	>	A
$*TC1$	I	>	H	>	G	>	F	>	E	>	D	>	C	>	B	>	A
$-BT$	I	=	C	>	H	=	D	>	G	=	F	>	E	>	B	>	A
BI	I	>	H	>	G	>	F	=	E	>	C	>	B	>	D	>	A
$*N_t$	I	>	H	>	G	>	F	>	E	>	D	>	C	>	B	>	A
$*twc$	I	>	H	>	G	>	E	>	F	>	D	>	C	>	B	>	A
wcx	I	>	H	>	E	>	F	>	G	>	B	>	C	>	A	>	D

One can observe that the six rather diverse symmetry-independent complexity indices (M_1 , M_2 , TC , $TC1$, N_t , twc) order nine graphs from Figure 1, starting with the most complex graph and ending with the least complex graph: I(6) > H(5) > G(5) > F(4) > E(4) > D(6) > C(6) > B(6) > A(6). Numerals in parentheses correspond to the number of times each structure was placed in the given position. For example, the numeral at I means that all six symmetry-independent complexity indices consider this graph to be the most complex one of the nine considered graphs.

In the case of symmetry-dependent complexity indices, there is no ordering supported by the majority of indices. Almost every index produces its

own ordering, which differs from the others. However, one symmetry-dependent complexity index (the *BT* index) gives the ordering of nine graphs that is roughly reverse to the ordering of other complexity indices. One might say that the *BT* index produces a kind of *simplicity* ordering of nine graphs by having the largest value for the simplest graph (A) out of the nine. But, it places last graphs C and I, both possessing the same value of the *BT* index. This does not agree with the rule that the cyclic structures are more complex than acyclic structures:^{22,26} Graph C is certainly simpler than I. The *BT* ordering given in Table II is based on the $-BT$ values. This is done to conform the *BT* ordering with orderings of other indices.

If we compare closely related symmetry-independent and symmetry-dependent complexity indices such as M_1 and SMM_1 , M_2 and SMM_2 , *twc* and *wcx*, the orderings they produce are different: M_1 and SMM_1 do not predict a single common placement, M_2 and SMM_2 predict only the common placements of I and F, and *twc* and *wcx* predict I and H as the most complex graphs out of the nine graphs considered and place I, H and C in the same position in their respective orderings. A problem with the symmetry-dependent complexity indices is that there is no unique way to introduce the influence of symmetry on the index. Of course, the ambiguity in ordering structures according to their complexity (or simplicity) could be resolved if there were a physical or a chemical property of molecules which could serve as a measure of molecular complexity. Unfortunately, no such property is known yet.²⁷

Following the rules²⁸ set by Bertz,^{4,22,29} Bonchev^{25,26,30–33} and others^{19,34} for hierarchical ordering of complex structures, the nine graphs from Figure 1 can be ordered as $I > H > G > F > E > D > C > B > A$. None of the six rules given in Ref. 28 allows the conclusion $F > E$. However, we ordered these two graphs in this way following the suggestion^{23,24} that a more complex graph has a greater number of connected subgraphs. The ordering of F and E really determines the balance between the influence of cycles (3- vs. 4-membered cycle) and side chains on their complexity. Thus it is by no means unreasonable to reverse these two graphs. Out of the 12 complexity indices reported in Table I, only *TC*, *TC1* and N_t produce orderings that entirely agree with the above ordering of the nine graphs. Out of the four Zagreb complexity indices, the ordering that the M_2 index produces is the closest to the above ordering except that the positions of E and F are reversed. The same ordering as by M_2 was also achieved by the *twc* index. The ordering produced by M_1 index is also close to the above ordering except that it gives $F = E$ and $D = C$ instead of $F > E$ and $D > C$.

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discussions about the complexity of molecules with A. T. Balaban (Bucuresti), S. C. Basak (Duluth, MN), S. H. Bertz (Mendham, NJ), D. Bonchev (Houston, TX) and M. Randić (Ames, IA). We thank D. Babić (Zagreb) for help in revising the manuscript, and Ch. Rücker (Freiburg) and reviewers for their critical, but helpful comments.

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14. A walk on a graph is an alternating sequence of vertices and edges beginning and ending with vertices, in which each edge is incident with two vertices immediately preceding and following it. A self-returning walk is a walk starting and ending at the same vertex.
15. Branching is an intuitive concept not uniquely defined (*e.g.*, J. W. Essam and M. E. Fisher, *Rev. Mod. Phys.* **42** (1970) 272–305), though it can be identified through the appearance of vertices of degrees three and higher.
16. One can look upon cyclicity as a kind of structural change resembling branching in that the values of degrees of some vertices within the cycle increase from two to three and higher at the sites of bridging cycle. This structural characteristic has been named (D. Bonchev, *Bulg. Chem. Comm.* **28** (1995) 567–582) an internal branching. Therefore, the degree of a vertex in a cycle can increase either by cyclization (the internal branching) or by attaching to it acyclic, cyclic or *spiro*-cyclic fragments (the external branching). These three possibilities correspond, for example, to cyclohexane \rightarrow bicyclo[2.2.0]hexane, cyclohexane \rightarrow isopropylcyclohexane and cyclohexane \rightarrow *spiro*[3.5]nonane.
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27. One of the three reviewers that we had for this article (Professor Douglas J. Klein, Texas A&M at Galveston, who allowed his name to be revealed) made interesting comments. Here we give his complete comments because they are very stimulating and of general interest.

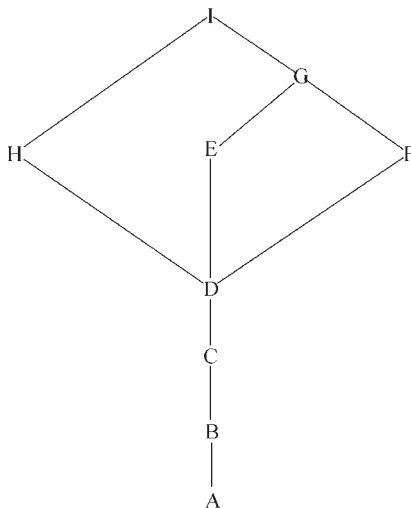
»This manuscript considers several topological indices as candidates for 'complexity measures' of graphs. These candidates are divided into two classes, six which are symmetry-independent and six (including a couple which are here considered for the first time) which are symmetry-attentive modifications. These various candidates are then tested on a suite of 9 representative molecular graphs to see if the complexity orderings are plausible.

There are a few relatively minor grammatical or stylistic problems, for which corrective suggestions are marked directly in the enclosed manuscript. But my primary comment is of a rather general (perhaps philosophical) nature. Indeed in chemistry (and elsewhere) there now and again is encountered a characteristic (such as 'complexity') to which various investigators ascribe different numerical values for the same molecule. Often the ambiguity in ascribed numerical values (say to 'complexity') does not seem to be due to imprecision in measured values – but rather the ambiguity is imagined to be due to some conceptual 'shortcoming' which if only rectified would lead to 'true' or 'correct' values for the particular characteristic. But there is another possibility - namely that such characteristics (as 'complexity') are not strictly numerical quantities. Perhaps many of these characteristics do not lead to a total ordering of the objects (*e.g.*, molecules) being so characterized. That is, the various ascriptions of numerical values of 'complexity' by different investigators would be just different partly faithful representations of an underlying 'complexity partial ordering'. In fact much of this philosophy has been espoused in a recent article by Klein and Babić (D. J. Klein and D. Babić, Partial Orderings in Chemistry, *J. Chem. Inf. Comput. Sci.* **37** (1997) 656–671), and some general ideas concerning posets as advanced that they seem tailor-made to the present circumstance involving 'complexity'. In particular in the present circumstance let S denote the ordered set of six symmetry-independent graph invariants,

$$S = \{M_1, M_2, TC, TC1, N_t, twc\}$$

with the i -th member ($i = 1 \rightarrow 6$) of this set denoted S_i . Then one may define a partial ordering relation \leq_S on the set of (connected) graphs such that two such graphs G_A & G_B are ordered as $G_A \leq_S G_B$ if $S_i(G_A) < S_i(G_B)$ for all $i = 1 \rightarrow 6$. In the nomenclature of Klein and Babić we then say that this resulting partial ordering is (if the set S is 'complete') a *mimic* for the fundamental complexity partial ordering. And there are several neat algebraic tools [described in sections 4 and 6 of Klein and Babić, as well as in an earlier article by Klein (D. J. Klein, Similarity

and Dissimilarity in Posets, *J. Math. Chem.* **18** (1995) 321–348)] which may be used to deal quantitatively with such 'scalable' posets, and such could be applied in the present circumstance of 'complexity'. Anyway, for the present case the 9 representative graphs (A, B, C, D, E, F, G, H, I) end up being partially ordered in consonance with the Hasse diagram (see Scheme 1).



Scheme 1

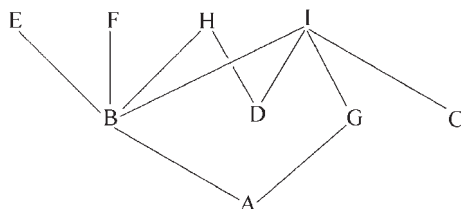
This diagram is such that in following downward along a path, say from species X to species Y , every one of the indices of the set S has a greater value for X than for Y (i.e., if $X \succeq_S Y$). Moreover, two species X and Y are directly connected by an edge downward from X to Y if and only if no third species may be placed (by this partial ordering) between X and Y . Evidently this diagram neatly presents in a pictorial fashion some relevant part of the detail recorded in Table II, and one quickly sees that the different indices of S all agree on the ordering of $I \succeq_S D \succeq_S C \succeq_S B \succeq_S A$ while the remaining species H, G, E, F always occur between I and D . Generally, one can ask (and perhaps answer) questions about this partial ordering in terms of such a (graph-like) Hasse diagram. For instance, it can be deduced that a set S' of just 3 numerical indices (in place of the set S of 6 indices) can be sufficient to induce the same Hasse diagram (or partial ordering) on the considered species.

One may of course follow the same approach for the set T of six symmetry-at-tentive graph invariants,

$$T = \{SMM_1, SMM_2, RCI, -BT, BI, wcx\}$$

where we have used $-BT$ instead of BT , so that it gives a closer degree of 'agreement' with the other invariants of this set. Then there is a partial ordering \leq_T of graphs, and the resultant Hasse diagram is in Scheme 2.

Clearly this is a less 'stringent' partial ordering than the first, and in agreement with the authors I think that the first set S leads to a better accordance with what might be called 'complexity'. The idea of 'stringency' here may be given a quanti-



Scheme 2

tative measure by considering the fraction f of pairs of graphs which turn out to be comparable under a given partial ordering (\leq_S or \leq_T). Then

$$f(\leq_S) = 32/36 = 8/9 = 0.89$$

and

$$f(\leq_T) = 15/36 = 5/12 = 0.42.$$

That is, \leq_S is much more nearly totally ordered (for which f would =1) than is \leq_T . Anyway, there are a number of different things that can be rather readily done, and I do think that »complexity« is partially ordered.

A further wide-ranging collection of original articles on chemical applications of partial orderings is scheduled to appear in volume **42** of *Communications in Mathematical and in Computer Chemistry (Match)*, to include a prolegomenon identifying well over 100 earlier relevant posetic references.«

28. The rules used are: (i) branched trees are more complex than unbranched trees; (ii) trees with several branches are more complex than trees with a single branch; (iii) cyclic structures are more complex than the corresponding acyclic structures; (iv) bicyclic structures are more complex than monocyclic structures; (v) branched cycles are more complex than cycles without branches and (vi) cycles with several external branches are more complex than cycles with a single branch.
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SAŽETAK**O zagrebačkim indeksima kao indeksima složenosti**

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Dva izvorna tzv. zagrebačka indeksa, označena kao M_1 i M_2 , uvedena 1972. godine, simetrijski su modificirana tako da su uzete u obzir jedino valencije vrhova (SMM_1) ili težine bridova (SMM_2) simetrijski ne-ekvivalentnih vrhova ili bridova grafa. Proučavana je njihova ovisnost o strukturnim odlikama i simetriji izabranih molekularnih grafova. Svi zagrebački indeksi ovise o strukturnim značajkama grafova, a indeksi SMM_1 i SMM_2 i o simetriji. Ta četiri zagrebačka indeksa uspoređena su s osam indeksa iz literature, i to na skupu od devet jednostavnih grafova s pet vrhova, koje su razmatrale i druge istraživačke skupine iz svijeta. Svaki razmatrani indeks dao je svoj poredak ovih grafova prema njihovoj složenosti. Samo tri indeksa iz literature daju potpuno identičan poredak razmatranih grafova. Poredak koji daje indeks M_2 podudara se s njima osim u redosljedu dvaju grafova, poredak koji daje indeks M_1 podudara se s njima u slučaju 7 grafova, dok se poretci koje daju SMM_1 i SMM_2 dosta razlikuju.