

On the Complexity of Platonic Solids*

Danail Bonchev

*Program for the Theory of Complex Natural Systems, Texas A&M University, Galveston, TX 77551, USA
(E-mail: bonchevd@sbcglobal.net, also: bonchevd@tamug.tamu.edu)*

RECEIVED APRIL 15, 2003; REVISED JULY 14, 2003; ACCEPTED JULY 14, 2003

Key words
Platonic solids
complexity
subgraph count
overall connectivity
overall Wiener
total walk count

Global, relative, and local complexity of the five Platonic solids (tetrahedron, octahedron, cube, icosahedron, and dodecahedron) are described and compared. Several of the most recent measures of topological complexity are used: the subgraph count, overall connectivity and overall Wiener indices, the total walk count, and the information theoretic index for vertex degrees distribution. Equations are derived for the first several orders of these indices as functions of the number of vertices and vertex degrees. Relative complexity, defined as the ratio of the complexity index selected and its value for the complete graphs having the same number of vertices as the respective Platonic solids, singles out tetrahedron as the most complex structure with 100 % relative complexity. The global complexity indices, as well as the local indices (defined per vertex and per edge) uniformly identify icosahedron as the most complex Platonic solid. These findings correlate with the preferable formation of icosahedron and tetrahedron in a variety of cases.

INTRODUCTION

Platonic solids attract the attention of scientists both with their high symmetry-based beauty and as models for crystal and molecular shapes. Assessments of Platonic solids topology and complexity were first initiated in the Zagreb research group of Professor Nenad Trinajstić.¹⁻⁵ The contributions of Prof. Trinajstić to the development of chemical graph theory are numerous and his important early papers in this area, on the Zagreb indices⁶ and their relations to molecular orbital theory⁷ and topological resonance energy,⁸ as well as his seminal monography,⁹ have attracted a plethora of researchers throughout the world to this fascinating area of theoretical chemistry. The present author also started his own journey in molecular topology during a three-month visit to Professor Trinajstić in 1976. This visit gave birth to a fruitful co-

operation between the Zagreb and Burgas groups of mathematical chemistry, which resulted in 19 joint papers published. These papers included the first detailed characterization of molecular branching¹⁰⁻¹² and molecular cyclicity¹³⁻¹⁹ patterns, along with their applications to QSPR/QSAR studies,²⁰⁻²⁵ and a combined topological/information-theoretical description of molecules.²⁶⁻²⁸

Quantitative assessments of the complexity of molecules and chemical reaction networks were first published in the 1980s,²⁹⁻³¹ although related studies on the complexity of graphs can be traced back another 10-15 years.^{32,33} Despite extensive studies and a number of rigorous complexity concepts proposed, the notion of complexity is still regarded by many as fuzzy and subjective. The present paper deals with what might be called structural or topological complexity. This kind of complexity can be unambiguously defined on a graph-theoretical ba-

* Dedicated to Professor Nenad Trinajstić on the occasion of his 65th birthday.

sis proceeding from relevant graph-invariants. The basic idea of structural complexity is that complexity increases with the number of structural elements and, particularly, with the number of their interactions. In graph-theoretical terms, the more vertices and edges a graph has, the more complex it is. More sophisticated complexity measures have been developed to describe the variety in the complexity of graphs having the same number of vertices and edges. Detailed information on complexity concepts and measures can be found in a recently published monograph.³⁴

The preceding complexity assessments of Platonic solids were made¹⁻⁵ with such topological indices as the Hosoya non-adjacency index,³⁵ the Randić connectivity index,³⁶ the number of spanning trees,^{1,2} the Bertz complexity index,^{29,30} the Estrada edge-connectivity index,³⁷ and Klein's resistance distances.^{3-5, 38-40} The present paper focuses on some recent complexity approaches based on the total subgraph count,⁴¹⁻⁴⁶ overall connectivity⁴⁴⁻⁴⁷ and overall Wiener⁴⁸ indices, and total walk count.⁴⁹⁻⁵²

Complexity Measures Used

The basic formulas used in calculations are briefly presented here. More details can be found in the references given in the foregoing introduction. A common feature of the subgraph count *SC*, overall connectivity *OC*, overall Wiener *OW*, and total walk count *TWC* indices is that they can be presented in a vector form $X(^0X, ^1X, ^2X, \dots, ^EX)$. Here, X is the global value the index has for the entire graph G , and E is the total number of edges in G :

$$X(G) = \sum_{k=1}^E {}^kX(G) \quad (1)$$

where ${}^kX(G)$ is the value of the respective k th-order complexity index $X(G)$. For the subgraph count, ${}^kSC(G)$ is simply the number of subgraphs kG_i having k edges. Similarly, ${}^kSWC(G)$ is the count of all walks of length k :

$${}^kSC(G) = \sum_i {}^kSC_i({}^kG_i \subset G) \quad (2)$$

$${}^kSWC(G) = \sum_i {}^kSWC_i({}^kG_i \subset G) \quad (3)$$

In the case of the k th-order overall connectivity kOC and overall Wiener kOW indices, the summing-up is taken over the values of a certain graph-invariant $X(G_i)$ in all subgraphs kG_i having k edges – the total subgraph adjacency $A_i({}^kG_i)$ for overall connectivity and the subgraph Wiener number $W_i({}^kG_i)$ for overall Wiener indices:

$${}^kOC(G) = \sum_i {}^kA_i({}^kG_i \subset G) \quad (4)$$

$${}^kOW(G) = \sum_i {}^kW_i({}^kG_i \subset G) \quad (5)$$

Besides the four measures of topological complexity given above, a topological-information complexity index, based on the vertex degrees distribution, I_{vd} , was

also tested. The index was defined⁵³ as the difference between the maximum value of Shannon's entropy, $H_{\max}(G)$, and the current entropy value $H(G)$ for the graph used to represent the respective Platonic solid:

$$I_{vd}(G) = \sum_{i=1}^V a_i \log_2 a_i \quad (6)$$

where a_i is the vertex degree and V is the number of vertices in the graph.

Equations (2–6) define global complexity measures. For comparative purposes one may also use relative measures, $X_r(G)$ or ${}^kX_r(G)$, obtained by dividing the global index X by the value that index has for the complete graph K_V having the same number of vertices V . Bertz and Herndon⁴¹ first used such an approach to calculate the complexity of molecules by finding their similarity to the most complex one having the same size. In the present paper, the k th order relative complexity index, ${}^kX_r(G)$, is similarly defined by dividing the k th order index ${}^kX(G)$ by the k th order of X in the respective complete graph:

$$X_r(G) = \frac{X(G)}{X(K_V)}; \quad {}^kX_r(G) = \frac{{}^kX(G)}{{}^kX(K_V)} \quad (7)$$

Due to the uniform vertex degrees in each Platonic solid (as well as in all regular or vertex-transitive graphs), the average complexity, defined per vertex and per edge, might also be regarded the local complexity of a vertex, $X(\text{vertex})$, or local complexity of an edge, $X(\text{edge})$:

$$X(\text{vertex}) = X(G) / V; \quad {}^kX(\text{vertex}) = {}^kX(G) / V \quad (8)$$

$$X(\text{edge}) = X(G) / E; \quad {}^kX(\text{edge}) = {}^kX(G) / E \quad (9)$$

Equations for the Complexity Indices of Platonic Solids

As seen from Eqs. (1–5), deriving closed-form equations for these complexity indices of Platonic solids (PS) would be a difficult task due to the presence of $E + 1$ terms in the *SC*, *OC*, and *OW* indices, and $V - 1$ terms in the *TWC* index. This is not necessary, however, because the first several terms of each of these measures suffice to assess and compare Platonic solids complexity. Derivations for these first terms are straightforward due to the fact that Platonic solids are represented by regular (and even vertex-transitive) graphs (Figure 1), which are graphs with vertices of identical degree a_i . The five solids will be abbreviated as T, O, C, I, D, for tetrahedron, octahedron, cube, icosahedron, and dodecahedron, respectively. While the equations for the first- and second-order indices are general for all Platonic solids and all vertex-transitive graphs, this is true of higher orders only for the total walk count. For this reason, the complexity of the five Platonic solids was assessed by two different equations for the third-order subgraph count,

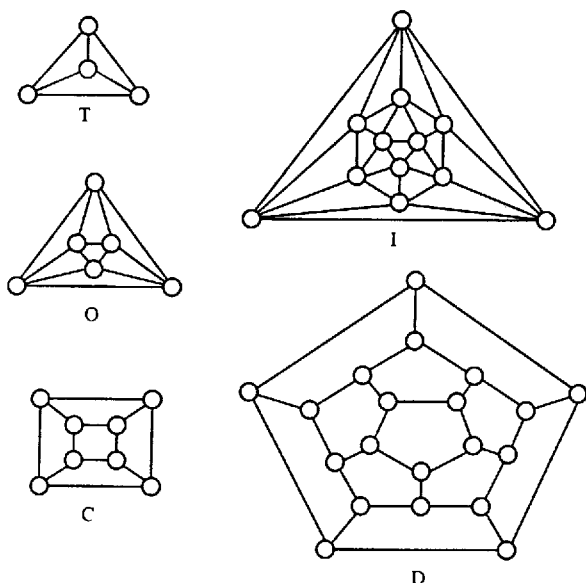


Figure 1. Schlegel graphs of the five Platonic solids: T – tetrahedron, O – octahedron, C – cube, I – icosahedron, D – dodecahedron.

overall connectivity, and overall Wiener indices. No expressions are shown for the first-order overall Wiener index and the first-order total walk count because they are directly related to the number of edges: ${}^1OW = E$; ${}^1TWC = 2E$. The details of the formulas' derivations for the third-order indices are given in the Appendix.

$${}^1SC(PS) = E = \frac{1}{2} V a_i \quad (10)$$

$${}^2SC(PS) = {}^1SC \times (a_i - 1) = \frac{1}{2} V a_i (a_i - 1) \quad (11)$$

$${}^3SC(T,O,I) = \frac{1}{6} V a_i (4a_i^2 - 9a_i + 1) \quad (12)$$

$${}^3SC(C,D) = \frac{1}{6} V a_i (a_i - 1) (4a_i - 5) \quad (13)$$

$${}^1OC(PS) = {}^1SC \times 2a_i = V a_i^2 \quad (14)$$

$${}^2OC(PS) = {}^2SC \times 3a_i = \frac{3}{2} V a_i^2 (a_i - 1) \quad (15)$$

$${}^3OC(C,D) = \frac{2}{3} V a_i^2 (a_i - 1) (4a_i - 5) \quad (16)$$

$${}^3OC(T,O,I) = \frac{1}{3} V a_i^2 (8a_i^2 - 18a_i + 1) \quad (17)$$

$${}^2OW = {}^2SC \times W(p2) = 2V a_i (a_i - 1) \quad (18)$$

$${}^3OW(C,D) = \frac{1}{2} V a_i (a_i - 1) (13a_i - 16) \quad (19)$$

$${}^3OW(T,O,I) = \frac{1}{2} V a_i (13a_i^2 - 29a_i - 2) \quad (20)$$

$${}^1SWC(PS) = 2E = V a_i \quad (21)$$

$${}^2SWC(PS) = {}^1SWC \times a_i = V a_i^2 \quad (22)$$

$${}^3SWC(PS) = {}^2SWC \times a_i = V a_i^3 \quad (23)$$

$$I_{vd}(PS) = V a_i \log_2 a_i \quad (24)$$

Obtaining relative complexity values of the Platonic solids (PS) requires preliminary derivation of equations for the complexity indices of the respective complete graphs K_4 , K_6 , K_8 , K_{12} , and K_{20} . However, with the exception of the third order SC , OC , and OW , Eqs. (10–24) can be directly transformed into equations for the indices of the respective complete graphs by substituting $a_i = V - 1$. The three different equations are shown below:

$${}^3SC(K_V) = \frac{1}{6} V (V - 1) (V - 2) (4V - 11) \quad (25)$$

$${}^3OC(K_V) = \frac{1}{6} V (V - 1)^2 (V - 2) (16V - 45) \quad (26)$$

$${}^3OW(K_V) = \frac{1}{2} V (V - 1) (V - 2) (13V - 38) \quad (27)$$

By writing down the relative complexity indices explicitly in Eq. (7), one immediately proves the equality of two pairs of such indices:

$${}^2SWC_r(PS) = {}^1OC_r(PS) = \frac{a_i^2}{(V - 1)^2} \quad (28)$$

$${}^2OW_r(PS) = {}^2SC_r(PS) = \frac{a_i (a_i - 1)}{(V - 1)(V - 2)} \quad (29)$$

It is noteworthy, that the approximate complexity measure of networks, called connectedness (Conn)^{53,54} or connectance (C),^{55,56} appears naturally in our scheme as a relative edge complexity E_r (or relative adjacency A_r):

$$E_r = \frac{E}{E(K_V)} = \frac{2E}{V(V - 1)} = \text{Conn} = \frac{A}{A(K_V)} = A_r \quad (30)$$

Equations for the local complexity indices (complexity of a vertex and complexity of an edge) can easily be obtained by substituting Eqs. (10–24) into Eqs. (8) and (9). One can thus find that the local edge connectivity E_V is half the vertex degree a_i :

$$E_V(G) = \frac{E}{V} = \frac{1}{2} a_i \quad (31)$$

DISCUSSION

The Platonic solids complexity indices were calculated by Eqs. (1–31) and verified with the computer software kindly made available by G. Rucker and C. Rucker.⁵⁷ The values obtained are shown in Tables I and II. The data for the global complexity indices, as well as from the direct comparison of the formulas derived, order the Platonic solids into the series $T < C < O < D < I$, thus defining the icosahedron as the most complex structure. The same conclusion about icosahedron was obtained by C. Rucker,⁵⁸ who used the number of cycles per vertex as a criterion, although the ordering of the five solids was different ($I > O > T > C > D$). Our ordering coincides entirely with the ones produced by the Bertz index,²⁹ and Estrada's second-order edge-connectivity index³⁷ reported by Trinajstić and coworkers.⁴ Classifying octahedron as more complex than cube (with six

TABLE I. Total and relative complexity measures of Platonic solids^(a)

Index	Tetra- hedron	Octa- hedron	Cube	Icosa- hedron	Dodeca- hedron
V	4	6	8	12	20
E	6	12	12	30	30
2SC	12	36	24	120	60
3SC	20	116	56	560	140
4SC	15	333	126	2730	360
1OC	36	96	72	300	180
2OC	108	432	216	1800	540
3OC	228	1824	672	11100	1680
4OC	180	6408	1872	67200	5400
2OW	48	144	96	480	240
3OW	168	1080	552	5340	1380
4OW	120	5640	2352	49680	6960
2TWC	36	96	72	300	180
3TWC	108	384	216	1500	540
4TWC	0	1536	648	7500	1620
I_{vd}	19.02	48	38.04	139.3	95.10
E_r	1	0.8	0.4286	0.4546	0.1579
2SC_r	1	0.6	0.1429	0.1818	0.0175
3SC_r	1	0.4462	0.0476	0.0688	0.0018
1OC_r	1	0.64	0.1837	0.2066	0.0249
2OC_r	1	0.48	0.0612	0.0826	0.0028
3OC_r	1	0.3577	0.0207	0.0312	0.0003
2OW_r	1	0.6	0.1429	0.1818	0.0175
3OW_r	1	0.45	0.0498	0.0686	0.0018
2TWC_r	1	0.64	0.1837	0.2066	0.0249
3TWC_r	1	0.512	0.0787	0.0939	0.0039
$I_{vd,r}$	1	0.6891	0.2420	0.3051	0.0589

^(a)The relative complexity indices are denoted by subscript «r». They are obtained by dividing the total index to the respective value for the complete graph having the same number of vertices V .

vs. eight vertices at the same number of eight edges) and, particularly, finding icosahedron to be more complex than dodecahedron (with twelve *vs.* twenty vertices at the same number of thirty edges) cannot be regarded as an artifact. Rather, it is a reflection of the higher local complexity; *i.e.*, the larger vertex degree in octahedron (four) and icosahedron (five), as compared to cube and dodecahedron (three). The same ordering of the five Platonic solids is preserved with the global values of the subgraph count, overall connectivity, and overall Wiener indices. As an illustration, the ordering according to the global SC values is shown: $T(64) < C(2441) < O(3705) < D(145,168,248) < I(964,957,974)$. However, the subgraph walk count restores the ordering to that dictated by the number of vertices: $T < O < C < I < D$: $156 (T) < 8,184 (O) < 26,232 (C) < 732,421,860 (I) < 34,867,843,980 (D)$, as do the Hosoya index,³⁵ the Randić (vertex-) connectivity index,³⁶ the Wiener index, and resistance distance.^{3-5,38}

TABLE II. Local (vertex and edge) complexities of Platonic solids

Index	Tetra- hedron	Octa- hedron	Cube	Icosa- hedron	Dodeca- hedron
E_v	1.5	2	1.5	2.5	1.5
2SC_v	3	6	3	10	3
3SC_v	5	19.33	7	46.67	7
4SC_v	3.75	55.5	15.75	227.5	18
1OC_v	9	16	9	25	9
2OC_v	27	72	27	150	27
3OC_v	57	304	84	925	84
4OC_v	45	1068	234	5600	270
2OW_v	12	24	12	40	12
3OW_v	42	180	69	445	69
4OW_v	30	940	294	4140	348
2TWC_v	9	16	9	25	9
3TWC_v	27	64	27	125	27
4TWC_v	0	256	81	625	81
$I_{vd,v}$	4.755	8	4.755	11.61	4.755
2SC_E	2	3	2	4	2
3SC_E	3.333	9.667	4.667	18.67	4.667
4SC_E	2.5	27.75	10.5	91	12
1OC_E	6	8	6	10	6
2OC_E	18	36	18	60	18
3OC_E	38	152	56	370	56
4OC_E	30	534	156	2240	180
2OW_E	8	12	8	16	8
3OW_E	28	90	46	178	46
4OW_E	20	470	196	1656	232
2TWC_E	6	8	6	10	6
3TWC_E	18	32	18	50	18
4TWC_E	0	128	54	250	54
$I_{vd,E}$	3.170	4	3.170	4.643	3.170

The relative complexity concept uses as a standard the complete graph having the same number of vertices as the structure under consideration. Indeed, tetrahedron, which is the smallest Platonic solid and which is described by a complete graph, now leads the series with 100 % complexity. The larger the Platonic solid, the lesser the chance for it to be close to the complete graph. The expectation that relative complexity will decrease in the series of Platonic solids with an increase in their number of vertices is violated only by the icosahedron, whose high local symmetry (vertex degree five) orders it before the cube: $T > O > I > C > D$.

The two kinds of average complexity assessments, complexity per vertex and complexity per edge (Eqs. 8 and 9), produce an ordering, $I > O > D \geq C \geq T$, close to that obtained with the global indices (the ordering of O and D is reversed). The equality signs refer to I_{vd} and the first several orders of the remaining complexity descriptors. For kSC , kOC , and kOW , the equality sign for

tetrahedron changes to inequality for $k = 3$, whereas $k = 4$ suffices to distinguish between cube and dodecahedron. When the subgraph walk count is averaged over vertices and edges, the equality is kept up to the last $(V - 1)$ term; *i.e.*, the distinction in ${}^k\text{SWC}$ between tetrahedron and the pair cube/dodecahedron occurs at $k = 4$, and the cube and dodecahedron are discriminated at $k = 8$.

One may thus conclude that (except for the global TWC index, which singles out dodecahedron) the global and local complexity descriptors SC , OC , and OW identify icosahedron as the most complex structure, whereas tetrahedron is the structure with the highest relative complexity.

The highest degree of complexity of tetrahedron and icosahedron, found in our study, is essential as an organizing principle of atoms and molecules into clusters, crystals, and supramolecular structures. Platonic solids are characterized by a minimum energy configuration, as compared to other solids having the same number and kind of atoms. The intra-cubic (\gg embeddable onto a cubic lattice \ll) polyhedrons tetrahedron, octahedron, and cube can fill 3D-space and form crystals. Importantly, the tetrahedral structure, which possesses a 100 % relative complexity, is the dominant crystal structure in the earth's crust. The extra-cubic dodecahedron and the icosahedron are non space-filling. However, in the liquid phase, spherical atoms

and molecules (*e.g.*, larger noble gases – argon, krypton, and xenon – as well as lead) prefer the clustering with the maximum global and local complexity – the icosahedral one. The latter has a lower Lennard-Jones energy than crystal structures but cannot form crystals due to the five-fold symmetry. Such five-fold symmetry is optimal for the short-range close packing but it is incompatible with the long-range order and favors amorphous structure.⁶⁰

The link between the solid geometry principles of Plato and Archimedes and the chemical assembly of small building blocks into large supramolecular structures has been used in the development of a general strategy for the construction of spherical molecular host systems (*e.g.*, liquid clathrates, macromolecular hosts). Icosahedron again has a central role in this »class of hosts for the new millennium.«⁶¹ Large atomic and molecular clusters also prefer icosahedral configuration. An extreme example of this class is the molecular packing in icosahedral viruses, including the HIV virus.⁶² Important correlations have been found between the virus crystal contacts and its biological function.

Acknowledgements. – Use of the software of G. Rucker and C. Rucker (Bayreuth) for calculating the SC , OC , OW , and TWC complexity descriptors is gratefully acknowledged. The author is indebted to Dr. C. Rucker, and the referees for their constructive criticism.

APPENDIX

The details of the derivation of the third-order complexity indices SC , OC , and OW are shown below. The numbering of the final equations corresponds to that in the basic text:

$${}^3\text{SC}(\text{path}(\text{C},\text{D})) = {}^2\text{SC} \times (a_i - 1) = \frac{1}{2} V a_i (a_i - 1)^2 \quad (\text{A1})$$

$${}^3\text{SC}(\text{path}(\text{T},\text{O},\text{I})) = {}^2\text{SC} \times \frac{2(a_i - 2) + (a_i - 1)(a_i - 3)}{a_i - 1} \\ = \frac{1}{2} V a_i (a_i^2 - 2a_i - 1) \quad (\text{A2})$$

$${}^3\text{SC}(\text{star}(\text{PS})) = V \times \frac{a_i!}{3!(a_i - 3)!} \\ = \frac{1}{6} V a_i (a_i - 1) (a_i - 2) \quad (\text{A3})$$

$${}^3\text{SC}(\text{triangle}(\text{T},\text{O},\text{I})) = \frac{1}{3} V a_i \quad (\text{A4})$$

$${}^3\text{SC}(\text{T},\text{O},\text{I}) = {}^3\text{SC}(\text{path}(\text{T},\text{O},\text{I})) + {}^3\text{SC}(\text{star}) \\ + {}^3\text{SC}(\text{triangle}) = \frac{1}{6} V a_i (4a_i^2 - 9a_i + 1) \quad (12)$$

$${}^3\text{SC}(\text{C},\text{D}) = {}^3\text{SC}(\text{path}(\text{C},\text{D})) + {}^3\text{SC}(\text{star}) \\ = \frac{1}{6} V a_i (a_i - 1) (4a_i - 5) \quad (13)$$

$${}^3\text{OC}(\text{C},\text{D}) = [{}^3\text{SC}(\text{path}(\text{C},\text{D})) + {}^3\text{SC}(\text{star}(\text{PS}))] \times 4a_i \\ = \frac{2}{3} V a_i^2 (a_i - 1) (4a_i - 5) \quad (16)$$

$${}^3\text{OC}(\text{T},\text{O},\text{I}) = [{}^2\text{SC}(\text{path}(\text{T},\text{O},\text{I})) + {}^3\text{SC}(\text{star}(\text{PS}))] \times 4a_i \\ + {}^3\text{SC}(\text{triangle}(\text{T},\text{O},\text{I})) \times 3a_i = \frac{1}{3} V a_i^2 (8a_i - 18a_i + 1) \quad (17)$$

$${}^3\text{OW}(\text{C},\text{D}) = {}^3\text{SC}(\text{path}(\text{C},\text{D})) \times W(p3) + {}^3\text{SC}(\text{star}(\text{PS})) \\ \times W(\text{star}) = \frac{1}{2} V a_i (a_i - 1) (13a_i - 16) \quad (19)$$

$${}^3\text{OW}(\text{T},\text{O},\text{I}) = {}^3\text{SC}(\text{path}(\text{T},\text{O},\text{I})) \times W(p3) + {}^3\text{SC}(\text{star}(\text{PS})) \\ \times W(\text{star}) + {}^3\text{SC}(\text{triangle}(\text{T},\text{O},\text{I})) \times W(\text{triangle}) \\ = \frac{1}{2} V a_i (13a_i^2 - 29a_i - 2) \quad (20)$$

In Eqs. (19 and 20), $p2$ and $p3$ stand for paths of length 2 and 3 edges, respectively.

REFERENCES

1. (a) N. Trinajstić, S. Nikolić, and Z. Mihalić, *Bull. Chem. Technol. Macedonia* **13** (1994) 61–68; (b) N. Trinajstić, S. Nikolić, D. Babić, and Z. Mihalić, *Bull. Chem. Technol. Macedonia* **16** (1997) 43–51.
2. S. Nikolić, N. Trinajstić, A. Jurić, Z. Mihalić, and G. Krilov, *Croat. Chem. Acta* **69** (1996) 883–897.
3. I. Lukovits, S. Nikolić, and N. Trinajstić, *Int. J. Quantum Chem.* **12** (1999) 217–225.
4. I. Lukovits, S. Nikolić, and N. Trinajstić, *Croat. Chem. Acta* **73** (2000) 957–967.
5. D. Babić, D. Klein, I. Lukovits, S. Nikolić, and N. Trinajstić, *Int. J. Quantum Chem.* **90** (2002) 166–176.
6. I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, *J. Chem. Phys.* **62** (1975) 3399–3405.
7. I. Gutman and N. Trinajstić, *Top. Curr. Chem.* **42** (1973) 49–93.
8. I. Gutman, M. Milun, and N. Trinajstić, *J. Am. Chem. Soc.* **1692**–1704.
9. N. Trinajstić, *Chemical Graph Theory*, 2nd ed., CRC Press, Boca Raton, FL, 1992.
10. D. Bonchev and N. Trinajstić, *J. Chem. Phys.* **67** (1977) 4517–4533.
11. D. Bonchev and N. Trinajstić, *Int. J. Quantum Chem. Symp.* **12** (1978) 293–303.
12. D. Bonchev, J. V. Knop, and N. Trinajstić, *MATCH* **6** (1979) 21–47.
13. D. Bonchev, O. Mekenyan, J. V. Knop, and N. Trinajstić, *Croat. Chem. Acta* **52** (1979) 361–367.
14. O. Mekenyan, D. Bonchev, and N. Trinajstić, *MATCH* **6** (1979) 93–115.
15. D. Bonchev, O. Mekenyan, and N. Trinajstić, *Int. J. Quantum Chem.* **17** (1980) 845–893.
16. O. Mekenyan, D. Bonchev, and N. Trinajstić, *MATCH* **11** (1981) 145–168.
17. O. Mekenyan, D. Bonchev and N. Trinajstić, *Int. J. Quantum Chem.* **19** (1981) 929–955.
18. O. Mekenyan, D. Bonchev, and N. Trinajstić, *Croat. Chem. Acta* **56** (1983) 237–261.
19. D. Bonchev and N. Trinajstić, *SAR QSAR Environ. Res.* **12** (2001) 213–235.
20. D. Bonchev, O. Mekenyan, G. Protic, and N. Trinajstić, *J. Chromatogr.* **176** (1979) 149–156.
21. D. Bonchev and N. Trinajstić, *Int. J. Quantum Chem. Symp.* **16** (1982) 463–480.
22. O. Mekenyan, D. Peitchev, D. Bonchev, N. Trinajstić, and I. Bangov, *Arzneim. Forsch.* **36** (1986) 176–183.
23. O. Mekenyan, D. Bonchev, N. Trinajstić, and D. Peitchev, *Arzneim. Forsch.* **36** (1986) 421–424.
24. O. Mekenyan, D. Peitchev, D. Bonchev, N. Trinajstić, and J. Dimitrova, *Arzneim. Forsch.* **36** (1986) 629–634.
25. O. Mekenyan, D. Bonchev, A. Sabljčić, N. Trinajstić, *Acta Pharm. Jugosl.* **37** (1987) 75–86.
26. D. Bonchev, G. Lickomannov, and N. Trinajstić, *Chim. Acad. Sci. Hung.* **102** (1979) 321–332.
27. O. Mekenyan, D. Bonchev, and N. Trinajstić, *Int. J. Quantum Chem. Symp.* **18** (1980) 369–380.
28. D. Bonchev, O. Mekenyan, and N. Trinajstić, *J. Comput. Chem.* **2** (1981) 127–148.
29. S. H. Bertz, *J. Am. Chem. Soc.* **103** (1981) 3599–3601.
30. S. H. Bertz, *J. Chem. Soc., Chem. Commun.* (1981) 818–820.
31. D. Bonchev, O. N. Temkin, and D. Kamenski, *React. Kinet. Catal. Lett.* **15** (1980) 119–124.
32. D. Minoli, *Atti Accad. Naz. Lincei, Cl. Sci. Fis. Mat. Nat. Rend. Ser. 8* **59** (1975) 651–661.
33. A. Mowshowitz, *Bull. Math. Biophys.* **30** (1968) 175–204.
34. D. Bonchev and D. H. Rouvray (Eds.), *Complexity in Chemistry*, Math. Chem. Ser. Vol. 7, Taylor & Francis, London, 2003.
35. H. Hosoya, *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.
36. M. Randić, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
37. E. Estrada, *J. Chem. Inf. Comput. Sci.* **35** (1995) 31–33.
38. D. J. Klein and M. Randić, *J. Math. Chem.* **12** (1993) 81–95.
39. D. J. Klein and O. Ivanciuc, *J. Math. Chem.* **30** (2001) 271–287.
40. D. J. Klein, *Croat. Chem. Acta* **75** (2002) 633–649.
41. S. Bertz and W. C. Herndon, in: *Artificial Intelligence Applications in Chemistry*, ACS, Washington, D. C., 1986, pp. 169–175.
42. S. H. Bertz and T. J. Sommer, *Chem. Commun.* (1997) 2409–2410.
43. S. H. Bertz and W. F. Wright, *Graph Theory Notes New York Acad. Sci.* **35** (1998) 32–48.
44. D. Bonchev, *Bulg. Chem. Commun.* **28** (1995) 567–582.
45. D. Bonchev, *SAR QSAR Environ. Res.* **7** (1997) 23–43.
46. D. Bonchev, in: J. Devillers and A. T. Balaban (Eds.), *Topological Indices and Related Descriptors*, Gordon and Breach, Reading, U.K., 1999, pp. 361–401.
47. D. Bonchev, *J. Chem. Inf. Comput. Sci.* **40** (2000) 934–941.
48. D. Bonchev, *J. Chem. Inf. Comput. Sci.* **41** (2001) 582–592.
49. G. Rücker and C. Rücker, *J. Chem. Inf. Comput. Sci.* **40** (2000) 99–106.
50. I. Gutman, C. Rücker, and G. Rücker, *J. Chem. Inf. Comput. Sci.* **41** (2001) 739–745.
51. G. Rücker and C. Rücker, *J. Chem. Inf. Comput. Sci.* **41** (2001) 1457–1462.
52. S. Nikolić, N. Trinajstić, I. M. Tolić, G. Rücker, and C. Rücker, in: D. Bonchev and D. H. Rouvray (Eds.), *Complexity in Chemistry*, Math. Chem. Ser. Vol. 7, Taylor & Francis, London, 2003, pp. 29–89.
53. D. Bonchev, in: M. Conn (Ed.), *Handbook of Proteomics Methods*, Humana, New York, 2003, pp. 451–462.
54. D. Bonchev, *SAR QSAR Environ. Res.* **14** (2003) 199–214.
55. D. J. Watts and S. H. Strogatz, *Nature* **393** (1998) 440–442.
56. H. Jeong, B. Tombor, R. Albert, Z. N. Oltval, and A. L. Barabasi, *Nature* **407** (2000) 651–654.
57. (a) G. Rücker and C. Rücker, *MATCH – Commun. Math. Comput. Chem.* **41** (2000) 145–149; (b) Unpublished programs SUBGRATCAU, SUBGRAOWAU, and MORGAN.
58. Note 15 in Ref. 49.
59. H. Wiener, (a) *J. Am. Chem. Soc.* **69** (1947) 17–20; (b) *J. Phys. Chem.* **52** (1948) 1082–1089.
60. M. Atiyah and P. Sutcliffe, *Milan J. Math.* (in press).
61. L. R. MacGillivray and J. L. Atwood, *Adv. Supramol. Chem.* **6** (2000) 157–183.
62. P. Natarajan and J. E. Johnson, *J. Struct. Biol.* **121** (1998) 295–305.