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Chemical applications of topology and group theory. 17. An information theoretical approach to polyhedral symmetry [1]

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Information theoretic parameters are described which measure the asymmetry of polyhedra based on partitions of their vertices, faces, and edges into orbits under action of their symmetry point groups. Such asymmetry parameters are all zero only for the five regular polyhedra and are all unity for polyhedra having no symmetry at all, i.e. belonging to the C_1 symmetry point group. In all other cases such asymmetry parameters have values between zero and unity. Values for such asymmetry parameters are given for all topologically distinct polyhedra having five, six, and seven vertices; all topologically distinct eight-vertex polyhedra having at least six symmetry elements; and selected polyhedra having from nine to twelve vertices. Effects of polyhedral distortions on these asymmetry parameters are examined for the tetrahedron, trigonal bipyramid, square pyramid, and octahedron. Such information theoretic asymmetry parameters can be used to order site partitions which are incomparable by the chirality algebra methods of Ruch and co-workers.

Key words: Information theory — Polyhedra — Symmetry — Asymmetry parameters

1. Introduction

Symmetry is an important property of chemically significant polyhedra. In this connection a variety of descriptors can be used to define the symmetry of polyhedra. The most conventional polyhedral symmetry descriptor uses the symmetry point group [2]. Using this approach an increase in the symmetry of a polyhedron leads to an increase in the size of its point group. A related symmetry descriptor uses the cycle index polynomial for all of the symmetry operations of the polyhedron in question [3]. An increase in symmetry leads to more terms in the cycle index polynomial.

Such symmetry descriptors may be regarded as additive since an increase in symmetry leads to an increase in the size of the symmetry descriptor, i.e. the point group or the cycle index polynomial. Other alternative symmetry descriptors are subtractive. Chirality algebra [4-6] provides an example of a subtractive symmetry descriptor since an increase in the symmetry of the system decreases the number of chiral site partitions.

This paper discusses a new type of subtractive symmetry descriptor also based on site partitions but having information theory [7, 8] rather than group representation theory [4, 9] as its mathematical basis. This approach represents an extension of work of Bonchev, Kamenski, and Kamenska [8] on the information content of chemical structures. The approach in this paper defines information theoretical *asymmetry parameters* for the vertices, edges, and faces of a polyhedron such that these parameters are all zero for the five regular polyhedra [10] and all unity for polyhedra having no symmetry, i.e. polyhedra having C_1 point group symmetry. These asymmetry parameters are functions solely of the site partitions of the vertices, the centers of the faces ("faces"), and the midpoints of the edges ("edges") of the polyhedron in question and in this sense have a similar genesis as the chirality functions [4, 5] arising from chirality algebra. However, the fact that the asymmetry parameters are always fractions ranging from zero for systems in which all sites of a given type (i.e. vertices, faces, or edges) are equivalent (i.e. in the same orbit of the symmetry point group) to unity in systems having no symmetry (i.e. each site of a given type is its own orbit in the C_1 point group) facilitates comparison of the symmetries of systems having radically different numbers of sites or symmetry point groups of different structures.

This paper defines such information theoretic asymmetry parameters for polyhedra. The values of these parameters are then examined for all polyhedra having seven or less vertices, all eight-vertex polyhedra having at least six symmetry elements, and selected polyhedra of chemical significance having nine through twelve vertices. Finally, this paper examines effects on such asymmetry parameters upon distortion of polyhedra of particular chemical importance: namely the tetrahedron, trigonal bipyramid, square pyramid, and octahedron.

2. Method

The polyhedron asymmetry parameters discussed in this paper are functions solely of the site partitions, where the sites are the vertices, the midpoints of the edges, or the midpoints of the faces. The site partitions are described by symbols of the type $(a_1^{b_1} a_2^{b_2} \cdots a_n^{b_n})$ where a_i and b_i are small positive integers and $a_i \geq a_{i+1}$ $(1 \leq i \leq n)$. In this symbol for the site partition there are b_i sets of a_i identical sites. The a_i identical sites correspond to an orbit of the symmetry group. Thus, if all of the N sites of a given type (i.e. vertices, faces, or edges) are equivalent, the site partition is represented as (N^1), abbreviated further as (N). Conversely, if all of the N sites of a given type are different (i.e. if there is no symmetry whatsoever), the site partition is represented as (1^N). For example, the site partitions of a trigonal bipyramid are (32) for the five vertices (i.e. three equatorial and two axial), (6) for the six (equivalent) faces, and (63) for the nine edges (i.e. six axial-equatorial and three equatorial-equatorial edges).

The information content of a site partition can be obtained from the following basic equation of Shannon [7]:

$$\bar{I} = -\sum_{i=1}^{n} p_i \lg p_i. \tag{1}$$

In Eq. (1), n is the number of orbits, p_i is the probability of the site being in orbit i, lg is a logarithm to the base 2, and $\bar{I}$ is the average information content per site. The probability p_i is obtained from the quotient N_i/N where N is the total number of sites and N_i is the number of sites in orbit i. For example, for the vertices of a trigonal bipyramid which correspond to a site partition (32),

$$\bar{I} = -(3/5)\lg(3/5) - (2/5)\lg(2/5) = 0.4422 + 0.5288 = 0.9710. \tag{2}$$

Note that if all of the sites are equivalent, there is only one orbit, the probability of being in the orbit is 1 so that the average information content per site is zero, i.e. $\bar{I} = -\lg 1 = 0$.

The maximum value of $\bar{I}$ for a collection of N sites occurs when all sites are different, i.e. the system has no symmetry so that each site is its own orbit. For such a fully asymmetric system

$$\bar{I}^0 = -\lg(1/N). \tag{3}$$

In Eq. (3) $\bar{I}^0$ represents the average information content per site for a fully asymmetric system. We can now define an asymmetry parameter A_s for N sites of type s (i.e. vertices, faces, or edges) by the quotient

$$A_s = \bar{I}/\bar{I}^0 \tag{4}$$

where $\bar{I}$ and $\bar{I}^0$ are defined as in Eqs. (1) and (3), respectively. For the vertices of a trigonal bipyramid with the site partition (32)

$$A_v(32) = \frac{-(3/5)\lg(3/5) - (2/5)\lg(2/5)}{-\lg(1/5)} = \frac{0.9710}{2.3221} = 0.4182. \tag{5}$$

Note that these asymmetry parameters depends only upon the site partitions. Furthermore, for N sites the asymmetry parameter for the fully symmetric site partition (N) is 0, that for the fully asymmetric site partition (1^N) is 1, and the asymmetry parameters for other site partitions fall between 0 and 1.

A further feature of the asymmetry parameter A_s defined in Eq. (4) is that for a given number of sites N, A_s can only have a finite number of discrete values, since there are only a relatively small number of ways for partitioning an integer

Table 1. Asymmetry parameters for topologically distinct polyhedra having five, six, and seven vertices

Point Group	Partitions Vertices	Faces	Edges	Asymmetry parameters Vertices	Faces	Edges	Federico number of dual	Comments
A) Five vertex polyhedra								
D_{3h}	(32)	(6)	(63)	0.4182	0	0.2897	#2	Trigonal bipyramid
C_{4v}	(41)	(41)	(4^2)	0.3109	0.3109	0.3333	#3	Square pyramid
B) Six vertex polyhedra								
O_h	(6)	(8)	(12)	0	0	0	#7	Octahedron
D_{3h}	(6)	(32)	(63)	0	0.4182	0.2897	#10	Trigonal prism
C_{5v}	(51)	(51)	(5^2)	0.2515	0.2515	0.3010	#6	Pentagonal pyramid
C_{2v}	(2^3)	(421)	$(4^2 21)$	0.6132	0.4911	0.5270	#8	
C_{2v}	(2^3)	(42^2)	$(4^2 21^2)$	0.6132	0.5000	0.5816	#4	Bicapped tetrahedron
C_2	(2^3)	(2^3)	$(2^4 1^2)$	0.6132	0.6132	0.7592	#9	
C_s	$(2^2 1^2)$	$(2^2 1^3)$	$(2^4 1^3)$	0.7421	0.7964	0.7898	#5	
C) Seven vertex polyhedra								
D_{5h}	(52)	(10)	(10, 5)	0.3074	0	0.2350	#23	Pentagonal bipyramid
C_{6v}	(61)	(61)	(6^2)	0.2108	0.2108	0.2789	#19	Hexagonal pyramid

C_{2v}	(421)	(2^3)	($4^2$21)	0.4911	0.6132	0.5270	#44	
C_{3v}	($3^2$1)	($3^2$1)	(3^4)	0.5161	0.5161	0.5578	#39, #40	Two isoentropic polyhedra
C_{2v}	(421)	(4$2^2$)	($4^2 2^2$1)	0.4911	0.5000	0.5843	#18	
C_{2v}	(421)	(2^4)	($4^2 2^2$1)	0.4911	0.6667	0.5843	#36	
C_{2v}	(421)	(4$2^2$1)	($4^2 2^3$)	0.4911	0.5794	0.5872	#16	
C_{3v}	($3^2$1)	($3^3$1)	(3^5)	0.5161	0.5706	0.5943	#12, #20	#20 = capped octahedron
C_{2v}	($2^3$1)	($4^2$2)	($4^2 2^3$1)	0.6947	0.4581	0.6246	#11	
C_2	($2^3$1)	($2^3$1)	(2^6)	0.6947	0.6947	0.7211	#41	
C_2	($2^3$1)	(2^4)	($2^6$1)	0.6947	0.6667	0.7506	#27, #37	
C_s	($2^2 1^3$)	($2^3 1^2$)	($2^6$1)	0.7964	0.7500	0.7506	#31	
C_2	($2^3$1)	(2^5)	($2^7$1)	0.6947	0.6990	0.7611	#13	
C_s	($2^3$1)	($2^2 1^3$)	($2^5 1^2$)	0.6947	0.7964	0.7675	#38	#35 and #38 are dual
C_s	($2^2 1^3$)	($2^3$1)	($2^5 1^2$)	0.7964	0.6947	0.7675	#35	#35 and #38 are dual
C_2 or C_s	($2^2 1^3$)	($2^4$1)	($2^6 1^2$)	0.7964	0.7196	0.7749	#14, #24	Two isoentropic polyhedra
C_s	($2^2 1^3$)	($2^3 1^3$)	($2^6 1^2$)	0.7964	0.7897	0.7749	#21, #22, #28	Three isoentropic polyhedra
C_s	($2^2 1^3$)	($2^2 1^2$)	($2^4 1^3$)	0.7964	0.7421	0.7898	#43	
C_s	($2^2 1^3$)	($2^3 1^2$)	($2^5 1^3$)	0.7964	0.7500	0.7921	#17, #29, #30	Three isoentropic polyhedra
C_1	(1^7)	(1^f)	(1^{f+7-2})	1.0000	1.0000	1.00000	#15, #25, #26,	Seven isoentropic polyhedra
		f = number of faces					#32, #33, #34, #42	With no symmetry

N into a sum of smaller integers, i.e., 5, 7, 11, 14, and 22 such partitions for $N = 4$, 5, 6, 7, and 8, respectively. For this reason, only in a small number of exceptional cases other than the fully symmetric $A(N) = 0$ and fully asymmetric $A(1^N) = 1$ can asymmetry parameters be matched for partitions of different numbers of sites. These relatively rare matching of asymmetry parameters for small values of N include $A(22) = A(422) = 0.5$ and $A(21^2) = A(2^3 1^2) = 0.75$.

A feature of the chirality algebra of Ruch and co-workers [4, 5] is the recognition of some sets of different partitions of n sites as *incomparable*. This occurs when two different partitions of the *same* number of sites are ordered differently by different, equaly valid, procedures. The simplest such pairs are the (3^2) and (41^2) partitions and the (2^3) and (31^3) partitions of six sites. The information theoretic asymmetry parameters for such incomparable site partitions may be distinct therby providing a basis for ordering site partitions which are incomparable by the methods of Ruch and co-workers [4, 5].

3. Results

The asymmetry parameters depend only on the site partitions and are given below for all possible partitions of four to eight sites:

A) Four Sites: $A(4) = 0$; $A(31) = 0.4057$; $A(2^2) = 0.5$; $A(21^2) = 0.75$; $A(1^4) = 1$.
B) Five Sites. $A(5) = 0$; $A(41) = 0.3109$; $A(32) = 0.4182$; $A(31^2) = 0.5905$; $A(2^2 1) = 0.6555$; $A(21^3) = 0.8278$; $A(1^5) = 1$.
C) Six Sites: $A(6) = 0$; $A(51) = 0.2515$; $A(42) = 0.3552$; $A(3^2) = 0.3868$; $A(41^2) = 0.4842$; $A(321) = 0.5645$; $A(2^3) = 0.6132$; $A(31^3) = 0.6935$; $A(2^2 1^2) = 0.7421$; $A(21^4) = 0.8711$; $A(1^6) = 1$.
D) Seven Sites: $A(7) = 0$; $A(61) = 0.2113$; $A(52) = 0.3075$; $A(43) = 0.3510$; $A(51^2) = 0.4093$; $A(421) = 0.4911$; $A(3^2 1) = 0.5161$; $A(32^2) = 0.5322$; $A(41^3) = 0.5929$; $A(321^2) = 0.6563$; $A(31^4) = 0.7580$; $A(2^2 1^3) = 0.7965$; $A(21^5) = 0.8378$; $A(1^7) = 1$.
E) Eight Sites; $A(8) = 0$; $A(71) = 0.1812$; $A(62) = 0.2704$; $A(53) = 0.3182$; $A(4^2) = 0.3333$; $A(61^2) = 0.3537$; $A(521) = 0.4329$; $A(431) = 0.4686$; $A(42^2) = 0.5$; $A(51^3) = 0.5163$; $A(3^2 2) = 0.5205$; $A(421^2) = 0.5833$; $A(3^2 1^2) = 0.6038$; $A(32^2 1) = 0.6352$; $A(41^4) = A(2^4) = 0.6667$; $A(321^3) = 0.7186$; $A(2^3 1^2) = 0.75$; $A(31^5) = 0.8019$; $A(2^2 1^4) = 0.8333$; $A(21^6) = 0.9617$; $A(1^8) = 1$.

Table 1 lists the asymmetry parameters for all topologically distinct polyhedra having five, six and seven vertices. The properties of these polyhedra are taken from Federico's extensive tabulation of polyhedra having from four to eight *faces* [11] by conversion of the polyhedra to their duals [12, 13]; the number of the dual of the polyhedron in question in Federico's table [11] is given to facilitate comparison. The polyhedra in Table 1 are ordered by increasing values of A_e, the edge asymmetry parameters, since among the three asymmetry parameters A_v, A_f, and A_e, the parameter A_e has the maximum number of possible values because a given polyhedron has more edges than either vertices or faces by Euler's theorem, i.e.

$$v + f = e - 2. \tag{6}$$

Table 2. Asymmetry parameters for topologically distinct polyhedra having eight vertices and at least six symmetry elements

Point Group	Partitions Vertices	Faces	Edges	Asymmetry parameters Vertices	Faces	Edges	Federico number of dual	Comments
O_h	(8)	(6)	(12)	0	0	0	#300	Cube
D_{6h}	(62)	(12)	(12, 6)	0.2704	0	0.2202	#54	Hexagonal bipyramid
T_d	(4^2)	(12)	(12, 6)	0.3333	0	0.2202	#49	Dual of truncated tetrahedron
D_{4d}	(8)	(82)	(8^2)	0	0.2173	0.2500	#172	Square antiprism
C_{7v}	(71)	(71)	(7^2)	0.1812	0.1812	0.2626	#247	Heptagonal pyramid
D_{2d}	(4^2)	(4^2)	(842)	0.3333	0.3333	0.3621	#287, #288	Two isoentropic polyhedra
D_{2d}	(4^2)	(82)	(84^2)	0.3333	0.2173	0.3750	#140	
D_{3d}	(62)	(6^2)	(6^3)	0.2704	0.2789	0.3801	#57	Bicapped octahedron
D_{3h}	(62)	(63)	(6^23)	0.2704	0.2897	0.3895	#245	3,3-bicapped trigonal prism
D_{2h}	(4^2)	(4^2)	(82^3)	0.3333	0.3333	0.4372	#282	Self-dual
D_{2d}	(4^2)	(84)	(84^22)	0.3333	0.2562	0.4404	#58	D_{2d}-dodecahedron
C_{3v}	(3^21^2)	(63)	(63^3)	0.6038	0.2897	0.4419	#191	Dual of triangular cupola
C_{3v}	(3^21^2)	(3^3)	(63^3)	0.6038	0.5000	0.4919	#194	

Table 3. Asymmetry parameters for selected polyhedra having nine to twelve vertices

Polyhedron	Point Group	Partitions Vertices	Faces	Edges	Asymmetry parameters Vertices	Faces	Edges
Tricapped trigonal prism	D_{3h}	(6, 3)	(12, 2)	(12, 6, 3)	0.2897	0.1554	0.3139
4-Capped square antiprism	C_{4v}	(4^21)	(8, 4, 1)	$(8, 4^3)$	0.4392	0.3348	0.4447
4,4-Bicapped square antiprism	D_{4d}	(8, 2)	(8^2)	(8^3)	0.2173	0.2500	0.3457
3,4,4,4,-Tetracapped trigonal prism	C_{3v}	(3^31)	(12, 3, 1)	$(12, 3^4)$	0.5706	0.2536	0.4362
$B_{11}H_{11}^{2-}$-polyhedron	C_{2v}	(42^31)	(4^32^3)	(4^52^31)	0.6321	0.6003	0.6417
Icosahedron	I_h	(12)	(20)	(30)	0	0	0
Cuboctahedron	O_h	(12)	(8, 6)	(24)	0	0.2588	0

Table 4. Asymmetry parameters of distorted polyhedra

Point Group	Partitions Vertices	Faces	Edges	Asymmetry Parameters Vertices	Faces	Edges	Comments
A) Distorted tetrahedra							
T_d	(4)	(4)	(6)	0	0	0	Regular tetrahedron
D_{2d}	(4)	(4)	(42)	0	0	0.3552	Loss of C_3 axis
C_{3v}	(31)	(31)	(3^2)	0.4057	0.5000	0.3868	Trigonal pyramid
C_{2v}	(2^2)	(2^2)	(41^2)	0.5000	0.5000	0.4842	Loss of C_3 and S_4 axes
C_s	(21^2)	(21^2)	(2^21^2)	0.7500	0.7500	0.7421	Reflection plane only
B) Distorted trigonal bipyramids							
D_{3h}	(32)	(6)	(63)	0.4182	0	0.2897	Maximum symmetry
C_{3v}	(31^2)	(3^2)	(3^3)	0.5905	0.3868	0.5000	Axial positions non-equivalent
C_{2v}	(2^21)	(42)	(42^21)	0.6554	0.3552	0.5794	Loss of C_3 axis
C_s	(21^3)	(2^21^2)	(2^31^3)	0.8277	0.7421	0.7897	Reflection plane only
C) Distorted square pyramids							
C_{4v}	(41)	(41)	(4^2)	0.3109	0.3109	0.3333	Maximum symmetry: square base
C_{2v}	(41)	(2^21)	(42^2)	0.3109	0.6554	0.5000	Rectangular base
C_{2v}	(2^21)	(41)	(42^2)	0.6554	0.3109	0.5000	Rhombus base

C_2	(2^21)	(2^21)	(2^4)	0.6554	0.6554	0.6667	Parallelogram base
C_s	(2^21)	(21^3)	(2^31^2)	0.6554	0.8278	0.7500	Trapezoid base
D) Distorted octahedra							
O_h	(6)	(8)	(12)	0	0	0	Regular octahedron
a) Three-fold axis (C_3) retained							
D_{3d}	(6)	(62)	(6^2)	0	0.2704	0.2789	"Trigonal antiprism
C_{3v}	(3^2)	(3^21^2)	(63^2)	0.3868	0.6038	0.4184	No σ_h
b) Horizontal symmetry plane (σ_h) retained; no three-fold axis (C_3)							
D_{4h}	(42)	(8)	(84)	0.3552	0	0.2561	Square cross-section
D_{2h}	(42)	(4^2)	(82^2)	0.3552	0.3333	0.3491	Rectangle cross-section
D_{2h}	(2^3)	(8)	(4^3)	0.6132	0	0.4421	Rhombus cross-section
D_2	(2^3)	(4^2)	(4^22^2)	0.6132	0.3333	0.5351	Parallelogram cross-section
C_{2v}	(2^3)	(42^2)	(4^221^2)	0.6132	0.5000	0.5741	Trapezoid cross-section
c) No horizontal symmetry plane (σ_h) or three-fold axis (C_3)							
C_{4v}	(41^2)	(4^2)	(4^3)	0.4842	0.3333	0.4421	Square cross-section
C_{2v}	(41^2)	(2^4)	(4^22^2)	0.4842	0.6667	0.5351	Rectangle cross-section
C_{2v}	(2^21^2)	(4^2)	(42^4)	0.7421	0.3333	0.6281	Rhombus cross-section
C_2	(2^21^2)	(2^4)	(2^6)	0.7421	0.6667	0.7211	Parallelogram cross-section
C_s	(2^21^2)	(2^21^4)	(2^51^2)	0.7421	0.8333	0.7676	Trapezoid cross-section

This, coupled with the intermediate dimensionality of edges (1) relative to vertices (0) and faces (2), suggests that A_e might be a better measure of polyhedral asymmetry than either A_v or A_f.

The asymmetry parameters of polyhedra having the common symmetry point groups fall into characteristic ranges. Thus the A_e values for polyhedra having the order 2 point groups C_s and C_2 fall in the range 0.7 to 0.8 whereas those having the order 4 point group C_{2v} fall in the range 0.5 to 0.65. Furthermore, since the asymmetry parameters depend only on site partitions, all three asymmetry parameters will be identical for two or more polyhedra having identical site partitions for their vertices, faces, and edges. Such a set of polyhedra can be called *isoentropic* because of the relationship of information content to entropy [14]. Examples of isoentropic seven-vertex polyhedra include the seven seven-vertex polyhedra having no symmetry; a set of three seven-vertex polyhedra with $A_v = 0.7964$, $A_f = 0.7897$, and $A_e = 0.7749$; a set of three seven-vertex polyhedra with $A_v = 0.7964$, $A_f = 0.7500$, and $A_e = 0.7921$; and four pairs of isoentropic seven-vertex polyhedra having A_e values of 0.5578, 0.5943, 0.7506, and 0.7749 (Table 1). For a pair of dual [12, 13] polyhedra P and P' (e.g. Federico dual numbers #35 and #38 in Table 1) $A_e = A'_e$, $A_v = A'_f$, and $A_f = A'_v$ in accord with the preservation of the symmetry of a polyhedron while constructing its dual.

According to Federico [11] the total number of combinatorically distinct eight-vertex polyhedra is 257, which is an intractable number for detailed study. However, if we exclude from consideration the large numbers of relatively uninteresting eight-vertex polyhedra having the relatively low symmetry point groups C_{2v}, C_2, C_s, and C_1, the remaining number of eight-vertex polyhedra drops drastically to 14, a manageable number but still including the eight-vertex polyhedra of greatest chemical interest [15]. Table 2 lists the asymmetry parameters of some nine- to twelve-vertex polyhedra that have arisen in chemical contexts.

A given polyhedron has three asymmetry parameters A_v, A_f, and A_e corresponding to the site partitions for the vertices, faces, and edges, respectively. All three of these parameters are zero only for the five regular polyhedra [10], namely the tetrahedron, octahedron (Table 1), cube (Table 2), icosahedron (Table 3), and regular (pentagonal) dodecahedron. Bipyramids, prisms, antiprisms, and the dual of the truncated tetrahedron (Table 2) have a single zero asymmetry parameter and the semiregular cuboctahedron [16] has zero values for A_v and A_e but not A_f.

Asymmetry parameters can also be used to follow the progress of distortion of relatively symmetrical polyhedra when symmetry elements are removed. Table 4 illustrates the effects of distortions on asymmetry parameters for four chemically significant polyhedra, namely the tetrahedron, trigonal bipyramid, square pyramid, and octahedron. Several different distortion pathways of the octahedron are examined in Table 4 depending on which symmetry elements (e.g. the C_3 axis or a σ_h symmetry plane) are destroyed first in the distortion process. Note that as symmetry elements are removed in these distortion processes, the values of the asymmetry parameters increase in accord with expectations.

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References

1. For part 16 of this series see King, R. B.: Theoret. Chim. Acta (Berl.) **64**, 453 (1984)
2. Cotton, F. A.: Chemical applications of group theory. New York: Wiley Interscience, 1971
3. King, R. B.: Inorg. Chem. **20**, 363 (1981)
4. Ruch, E., Schönhofer, A.: Theoret. Chim. Acta (Berl.) **10**, 91 (1968)
5. Ruch, E.: Acc. Chem. Res. **5**, 49 (1983)
6. King, R. B.: Theoret. Chim. Acta (Berl.) **63**, 103 (1983)
7. Shannon, C., Weaver, W.: Mathematical theory of communication. Urbana: University of Illinois, 1949
8. Bonchev, D., Kamenski, D., Kamenska, V.: Bull. Math. Biol. **38**, 119 (1976)
9. Gorenstein, D.: Finite groups. New York: Harper and Row 1968
10. Hilbert, D., Cohn-Vossen, S.: Geometry and the Imagination. New York: Chelsea 1952
11. Federico, P. J.: Geom. Ded. **3**, 469 (1975)
12. Grunbaum, B.: Convex polytopes. New York: Interscience 1967
13. R. B. King. In: Chemical applications of topology and graph theory. King, R. B. (ed.) Amsterdam: Elsevier Scientific Publishing Company 1983
14. Fast, J. D.: Entropy. Eindhoven: Philips 1968
15. Kepert, D. L.: Prog. Inorg. Chem. **24**, 179 (1978)
16. Lyusternik, L. A.: Convex Figures and Polyhedra. New York: Dover 1963