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Similarity and complexity of the shapes of square-cell configurations

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Summary. An equivalence relation on square-cell configurations, which we call animals, is formulated precisely, using the similarity criterion of "seeing" parts of the shape of the animal from its interior, and an operation called "squashing", leading to a smaller animal. It is noted that there is a unique smallest animal in each resulting equivalence class, called the canonical animal of its class. It is proposed that the number of cells in a canonical animal A serves as a measure of complexity of any animal similar to A. The formulation of the canonical animal is suggested as a tool for characterizing shapes of monolayer clusters of adsorbed molecules on square lattices, a problem of importance in chemical catalysis.

Key words: Shape analysis – Lattice animals – Similarity – Complexity

1. Introduction

The characterization of shapes of two-dimensional domains on a plane is of importance in both pure and applied mathematics, and in most of the natural sciences. For example, the shapes of molecular clusters adsorbed on the surface of a metal catalyst are of major importance in chemistry. Many of the essential aspects of this problem can be studied by modeling the molecules by square-cell configurations which we call *animals*. The animals with at most five cells are shown in Fig. 1. We are interested in the intrinsic shapes of animals and in the present study we shall not distinguish between animals that are mirror images, or generated by rotation from each other. These rotated and reflected versions will be considered as different placements of the same animal A. The problem of determining the exact number of animals with n cells is discussed in [1]. Statistical properties of animals and their embeddings in lattices are important in modeling a variety of physical problems [2, 3]. There is a need for efficient techniques for describing and comparing the shapes of animals. A simple technique will be proposed for this purpose, based on the novel concepts of similarity and complexity measure of animal shapes which we now develop.

To facilitate the development of our complexity measure, an intuitive description of the conceptual framework will be given. The concepts listed below

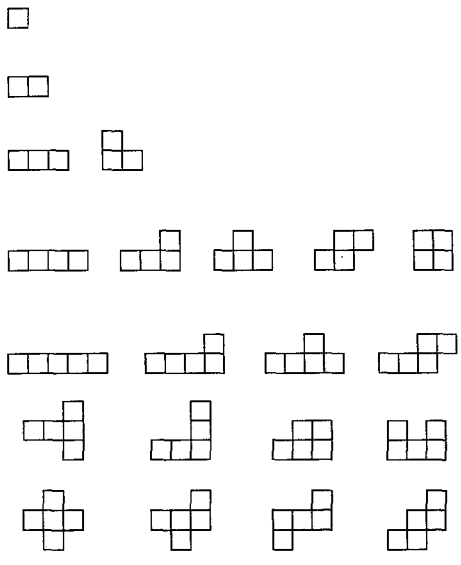

Fig. 1. List of square-cell configurations (animals) of five cells or less. Animals related to one another by rotation or reflection are regarded equivalent and only one animal is listed from each equivalence class

appear in [4]. A point u inside a Jordan curve J in the plane is said to *see* that part of J consisting of all points x of J for which the interior of the straight line segment ux contains no point of J. A *seeing basis* B for seeing J is a set of points in the interior of J such that B sees J and for each point $u \in B$, the subset $B - u$ does not see all of J. Thus each seeing basis B is a minimal set of points that see J, in the sense that no proper subset of B will do. A *minimum seeing basis* B for J is a seeing basis B such that no other basis B' contains fewer points, i.e., $|B| \leqslant |B'|$. We shall study the shape features and simple transformations (called squashing) of special Jordan curves which can be treated by the techniques of graph theory, where the seeing properties of certain subgraphs (called maximal submeshes) are not altered by the transformations.

It is possible to approximate the interior of a Jordan curve by a family of inscribed squares of uniform size. These families of squares can be regarded as square-cell animals, and the problem of seeing a Jordan curve J suggests a connection with characterizing the shape of animals.

Animals are definable as certain subgraphs of a mesh. By definition [5], the *mesh* $M_{(m,n)}$ is the cartesian product $P_m \times P_n$ of two nontrivial paths P_m and P_n. When $m = n$, then we write $M_{(n)}$ for the mesh $P_n \times P_n$ (see Fig. 2). The *interior* of a given drawing of a graph G in the plane is the union of open point sets enclosed by the cycles of G. A *simply connected subgraph* S of a mesh M has no holes, that is, each node v and each cell c of the mesh M falling within the interior of S is also a node and a cell, respectively, of S. We follow the graph

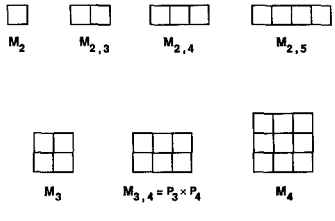

Fig. 2. Some of the simple meshes. A mesh $M_{(m,n)}$ is defined as the cartesian product $P_m \times P_n$ of two nontrivial paths P_m and P_n

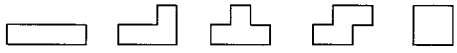

Fig. 3. The Jordan curves associated with the five four-cell animals of Fig. 1

theoretic notation and terminology of [6, 7]. A *block* is a connected graph with no cutnodes. Since our goal is shape characterization of simply connected square-cell configurations in the plane, it is useful to define lattice animals in terms of Jordan curves on a lattice. A *Jordan cycle* C of a mesh $M_{(n)}$ is a cycle that is a subgraph of mesh $M_{(n)}$ and has a vertex degree of two for all of its nodes [8]. A subgraph A of mesh $M_{(n)}$ is an *animal* if A contains precisely all the edges and nodes of $M_{(n)}$ that fall on or within the interior of some Jordan cycle C of mesh $M_{(n)}$ [8]. As implied by this definition, each animal A is a simply connected block. Although this definition is limited to simply connected entities, one should note that in a different context it is often useful to extend this definition to multiply connected arrangements. In the literature lattice animals are often allowed to be multiply connected. However, in this study we shall not be concerned with such generalizations.

Each 4-cycle C_4 contained in A is called a *cell* c of A. The *perimeter* of A contains all edges of A which are on exactly one cell. Thus the perimeter of A is the Jordan cycle C defining the animal; hence, as a point set, it is a single Jordan curve $J(A)$. The Jordan curves associated with the 4-cell animals are listed in Fig. 3. Clearly, every 4-cycle inside the perimeter of an animal A is a subgraph of A.

The problem of seeing a Jordan curve J is trivially simple if the curve is a convex polygon, since then every seeing basis consists of just a single point, which may be arbitrarily chosen inside J. Among convex polygons, rectangles have the simplest properties. Rectangles can be approximated very simply by a family of squares ordered into rows and columns. Some of these squares can be regarded as cells of animals; hence it is natural to consider the mesh and various submeshes of animals as tools of shape characterization of both the animals themselves and the Jordan curves related to the animals by some approximate representation.

2. Animal codes

The (circumscribed) *mesh* $M(A)$ *of an animal* A is the unique smallest mesh $M_{(m,n)}$ containing A as a subgraph. Thus animal A can be represented as a rectangular $(m-1) \times (n-1)$ matrix $R(A) = [r_{ij}]$ where $r_{ij} = 1$ if the i,j-cell of mesh $M_{(m,n)}$ is a cell of A, while $r_{ij} = 0$ otherwise, as introduced in [7]. Recall that we shall not distinguish between animals that are mirror images or can be obtained from each other by rotations in the plane as we are primarily interested in their intrinsic shape features. The chirality properties of square-cell configurations are discussed elsewhere [8]. However, the freedom in rotations and reflections of the $M(A)$, A pair in the plane lead to additional matrix representations. Figure 4 shows an animal A, its mesh $M(A)$ and the corresponding matrix $R(A)$. Obviously, a matrix $R(A)$ need not be unique, as shown in Fig. 5 where $R_1(A)$ and $R_2(A)$ and their transposes $R_i'(A)$ are all different matrices obtained from the same animal A.

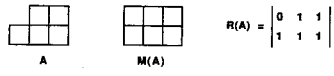

Fig. 4. Example for an animal A, its mesh $M(A)$, and matrix $R(A)$

$$R_1(A) = \begin{vmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \end{vmatrix} \qquad R_2(A) = \begin{vmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \end{vmatrix}$$

Fig. 5. Alternative matrices for animal A of Fig. 4

These considerations suggest a code $c(A)$ for an animal A. For each animal A, there are four possible R-matrix pairs, where the two matrices in each pair are the transposes of each other. In the case of an $m \times n$ mesh of A, illustrated for $m-1=2$, these matrices can be given as follows, where φ_1 is the binary string which is row 1 of matrix R_1 and φ_2 is row 2 of R_1:

$$R_1 = \begin{vmatrix} \varphi_1 \\ \varphi_2 \end{vmatrix}, \quad R_2 = \begin{vmatrix} \varphi_2 \\ \varphi_1 \end{vmatrix}, \quad R_3 = \begin{vmatrix} \sigma_1 \\ \sigma_2 \end{vmatrix}, \quad R_4 = \begin{vmatrix} \sigma_2 \\ \sigma_1 \end{vmatrix},$$
$$R_5 = R_1', \quad R_6 = R_2', \quad R_7 = R_3', \quad \text{and } R_8 = R_4'. \tag{1}$$

Matrix R_2 has φ_1 and φ_2 interchanged, exactly as in Fig. 5. Symbol σ_1 is used to denote the reverse of row 1; for example, row 1 in $R(A)$ of Fig. 4 is the reverse of φ_1 of $R_1(A)$ in Fig. 5: 0 1 1 compared with 1 1 0. In general, matrices R_2 and R_4 contain the rows $1, 2, \ldots m-1$ of matrices R_1 and R_3, respectively, in reversed order, $m-1, \ldots 1$. For example, when an animal A has a matrix with three rows,

$$R_1(A) = \begin{vmatrix} \varphi_1 \\ \varphi_2 \\ \varphi_3 \end{vmatrix}$$

then the other matrices are

$$R_2 = \begin{vmatrix} \varphi_3 \\ \varphi_2 \\ \varphi_1 \end{vmatrix}, \quad R_3 = \begin{vmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \end{vmatrix}, \quad R_4 = \begin{vmatrix} \sigma_3 \\ \sigma_2 \\ \sigma_1 \end{vmatrix},$$
$$R_5 = R_1', \quad R_6 = R_2', \quad R_7 = R_3', \quad \text{and } R_8 = R_4'.$$

Note that, not all of the eight matrices are necessarily different.

The *binary number* $b(R_1)$ of the binary matrix R_1 is the concatenation $\varphi_1 \circ \varphi_2$. Thus for $R_1(A)$ in Fig. 5 we have $b(R_1(A)) = 110111 = 55$. In general, the binary number $b(R)$ of R is obtained by concatenation of the rows of R. We can now define the *code* $c(A)$ of an animal A as follows:

$$c(A) = \max\{b(R_i), i = 1, 2, \ldots, 8\}. \tag{2}$$

This gives $c(A) = 111110 = 62$ for the code of animal A of Fig. 4, as given by matrix $R_2(A)$ of Fig. 5.

Note that if the number of rows differs from the number of columns then the matrix representation $R_i(A)$ for which $b(R_i) = c(A)$ and the corresponding placement of A are not necessarily unique. In the example, the transpose $R_2'(A) = R_6(A)$ of $R_2(A)$ has the same binary number b, $b(R_6) = b(R_2) = c(A)$, and the two placements of A and the corresponding two matrices realize the code $c(A)$. We shall choose a standard placement for each animal A, a placement that has a matrix representation $R_i(A)$ with binary number $b(R_i)$ equal to the code $c(A)$ of A.

In general, we chose the *standard placement* of the animal A as the one that corresponds to the code generating matrix $R_i(A)$ $[b(R_i) = c(A)]$ if this matrix is unique, and if there are two different matrices generating the code, then we take the one that has fewer rows than columns, $m < n$; there can exist at most two different matrices with the same maximal binary number $b(R_i) = c(A)$, and if there are two such matrices, then one of them must have $m < n$, the other $m > n$.

In the above example, this choice leads to $R_2(A)$ of Fig. 5 as the matrix corresponding to the standard placement of A. In general, the condition $m < n$ leads to a unique choice of placement, since if two or more rotated or reflected versions of the same animal A have the same binary number $b(R_i)$, while $m < n$ for each, then all these placements are indistinguishable, and hence are regarded as being the same. For example, "Skinny", the first four-cell animal listed in Fig. 1, is shown in its standard placement, having matrix $R_i(A) = (1, 1, 1, 1)$ and code $c(A) = 1111$. This placement is indistinguishable from all those obtained by vertical or horizontal reflections or 180° rotations, and these are precisely the placements which have the same binary number $b(R_i) = (1, 1, 1, 1)$ and fulfill the condition $m < n$ for their matrices. For "Fatty", the last four-cell animal in Fig. 1, all rotated and reflected versions are indistinguishable from one another, all matrix representations are equivalent, and hence there is only one matrix, $R = R_i = R_j$, and $c(A) = b(R_i)$, $i, j = 1, 2, \ldots, 8$.

The code $c(A)$ itself does not completely determine the animal A as the values of m and n are also needed in order to determine the circumscribed mesh $M(A)$ of A. For example, the code $c(A) = 1111$ may be that of Skinny or Fatty. Note, however, that $c(A)$ and the number of rows $m - 1$ determines n. (At least $m - 1$ zeroes would be required to be placed in front of the binary code $c(A)$ in order to increase the number of columns of the matrix and decatenate the code in a different way, leading to a different animal; however, the first row of the matrix realizing the code must start with fewer than $(m - 1)/2$ zeroes, otherwise another placement would have a greater binary number.) Consequently, a determining numerical invariant $i(A)$ of any animal A is the ordered pair, in which $c = c(A)$:

$$i(A) = (c, m). \tag{3}$$

If $d(c)$ is the number digits in the binary number c, then the number n of columns is equal to $d(c)/(m - 1)$ if this is an integer, otherwise $n = \text{int}[d(c)/(m - 1)] + 1$.

3. Similarity and complexity of animal shapes

Now we turn to the specification of the shape of an animal A by means of a precise equivalence called shape similarity, or simply, similarity for brevity. A *maximal submesh* M of A is a subgraph of A which is a mesh not contained in any larger submesh of A. Clearly, every animal A has a well-defined set of maximal submeshes. For convenience and without any ambiguity, we identify

$$\text{N} = \text{north} = \text{top}, \quad \text{W} = \text{west} = \text{left}, \quad \text{S} = \text{south} = \text{bottom} \quad \text{E} = \text{east} = \text{right}.$$

The symbol X will be used for a general direction, $X \in \{\text{N}, \text{W}, \text{S}, \text{E}\}$. The direction obtained from X by a counterclockwise rotation of 90 degrees is denoted by X', for example, $\text{N}' = \text{W}$, $\text{N}'' = \text{S}$, and $\text{N}''' = \text{E}$. Animal A of Fig. 4 has two maximal submeshes: $M_{(2,4)}$ at its south and $M_{(3)}$ at its east.

By definition, a *line of a mesh* $M_{(m,n)}$ is a row of $m - 1$ cells or a column of $n - 1$ cells of the mesh. The X-line of a mesh M is the family of all cells on the

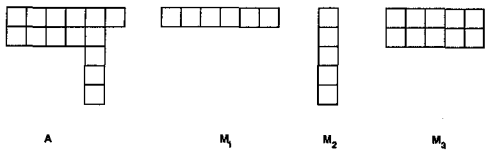

Fig. 6. Example of an animal A, and its three maximal submeshes, M_1, M_2, and M_3.

X-side of M. The $(X-1)$-line of M is the X-line of the mesh obtained from M by removing its X-line. The $(X-k)$-line of M is defined by recursion.

Below we describe a process for contracting a given animal A to a smaller animal of similar shape. We do this by diminishing a maximal submesh of A when possible, while preserving the essential shape features of A. This process will be called *squashing* and will be accomplished in stages by operations called *elementary squashings*. An elementary squashing is accompanied by the *fusion* of certain cells. We illustrate the procedure before stating it precisely, using the example of animal A in Fig. 6. Animal A has three maximal submeshes M_1, M_2 and M_3. Each submesh has four sides, its N-line, W-line, S-line, and E-line, in the directions of N, S, W, and E, respectively.

Stated informally, the fusion of two neighboring cells c_1 and c_2 of an animal A is the replacement of the two cells by a new cell c_3, so that along the X, X'' directions defined by the two cells their neighbor relations with any other cells of A are inherited by c_3. Formally, this may be stated as follows: *Fusion* of two cells c_1 and c_2 of an animal A, where c_2 is the X-neighbor of c_1 for direction X, occurs when the pair c_1 and c_2 are replaced by a cell c_3, so that the X-neighbor of c_2 and the X''-neighbor of c_1 become the respective X- and X''-neighbors of cell c_3 in the resulting new animal. Before fusion, the two cells have six edges available for neigbor relations with additional cells, whereas the new, fused cell has only four edges. Whether two neighbor cells are fusible or not depends on the local and global pattern of neighbor relations among the cells.

Cells c_1 and c_2 of an animal A are *locally fusible* if c_2 is the X-neighbor of c_1 for some direction X, and both of the X' and X''' edges of the cells c_1 and c_2 are on the perimeter of A. If several fusions are carried out simultaneously, then certain cell pairs that are not locally fusible still can be fused, since fusion of some neighboring cells may eliminate some neighbor relations which prevent fusion of individual pairs.

In order to squash a submesh, we need to fuse pairs of lines of the submesh. Such an operation is not always feasible. For example, if an additional cell c exists at the X' end of the $(X-1)$-line of a submesh M of an animal A, then identifying the X-line with the $(X-1)$-line could not lead to another animal, since the neighbor relation of c with the X' end of the new X-line would be undecided.

Two families $\{c_{1i}, i=1,k\}$ and $\{c_{2i}, i=1,k\}$ of cells of an animal A are simultaneously fusible if there exists a common direction X such that in each pair c_{1i}, c_{2i}

(i) the cell c_{2i} is the X-neighbor of c_{1i},

(ii) the pair of X'-edges of c_{1i} and c_{2i} is either on the perimeter of A or is a pair of X'''-edges of another c_{1j} and c_{2j} pair from the respective families,

(iii) the pair of X'''-edges of c_{1i} and c_{2i} is either on the perimeter of A or is a pair of X'-edges of another c_{1j} and c_{2j} pair from the respective families.

A special case of simultaneous fusion applies to lines of certain maximal submeshes.

A maximal submesh M of A is *X-fusible* if it has an $(X-k)$-line and an $(X-k-1)$-line and if the X' and X''' cells of both the $(X-k)$-line and $(X-k-1)$-line of M are on the perimeter of A. These lines are called X-fusible line pairs of M. The process of X-fusing an X-fusible maximal submesh M of A is defined as the simultaneous fusion of each cell c of an $(X-k)$-line with the cell c'' on its X'' side, where the pair $(X-k)$-line and $(X-k-1)$-line of M is an X-fusible line pair.

A maximal submesh M of A is *X-squashable* if M is X-fusible, and X-fusing M

(i) converts M into a maximal submesh M' of a square cell configuration that is still an animal,

(ii) leaves the number of maximal submeshes invariant.

A nontrivial *elementary squashing* (*elementary X-squashing*) of an animal A is the X-fusing of an X-squashable maximal submesh M of A. The trivial elementary squashing of A (no squashing) does not alter A. For example, animal A of Fig. 4 admits only one nontrivial elementary squashing, namely, the removal of the two easternmost cells of A, resulting in the second 3-cell animal of Fig. 1.

In order to define a sequence for elementary squashings, we shall order the maximal submeshes M_j of the animal. Take the matrix representation $R_i(A)$ of the standard placement of the animal A, retain only those matrix elements which correspond to the cells of M_j and replace all other elements with 0. Concatenation of the rows of the resulting matrix defines a binary code $c(M_j)$ of the maximal submesh M_j of A. In the standard placement of the animal A each maximal submesh M_j has a unique code $c(M_j)$. The maximal submeshes of A are ordered according to the decreasing order of their codes. The *primary squashable maximum submesh* M_1 of A is the squashable submesh of greatest binary code $c(M_j)$.

A *squashing* of an animal A is a sequence of elementary squashings, generating a finite sequence of animals, where in each step the number of cells of the animals decrease. In each step an elementary squashing is carried out on the primary squashable maximal submesh M_1 of the current animal. The elementary squashing is performed at the N-fusible pair of $(N-k)$- and $(N-k-1)$-lines of smallest possible k value along the N direction of the standard placement of the current animal if M_1 is N-squashable. Otherwise the elementary squashing is carried out at the W-fusible pair of $(W-k)$- and $(W-k-1)$-lines of smallest possible k value along the W direction of the standard placement. Since M_1 is squashable, it must be squashable along at least one of these two directions. The procedure is repeated for the new animal obtained. Starting from a given animal A, the sequence of elementary squashings and that of the animals obtained are well defined.

Now, two animals A_1 and A_2 are *shape-similar* (or more briefly, *similar*) if there is an animal A which can be obtained from both A_1 and A_2 by squashings. Obviously, similarity is an equivalence relation since it is reflexive, symmetric and transitive.

An animal which has no nontrivial elementary squashing is called *irreducible*. Clearly, every animal A is similar to a unique irreducible animal A°. We say that A° is the *canonical form* of A. In Fig. 7 a squashing sequence of two elementary squashings of animal A of Fig. 6 is shown, leading to the canonical form A°. Figure 8 shows the irreducible animals taken from Fig. 2.

The number of n-cell animals will be denoted a_n and the number of those which are irreducible by c_n; Table 1 gives the values of a_n and c_n for $n \leqslant 5$.

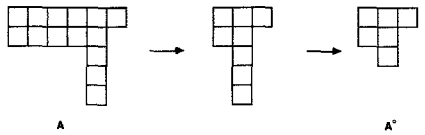

Fig. 7. A squashing of animal A of Fig. 6 by a sequence of two elementary squashings

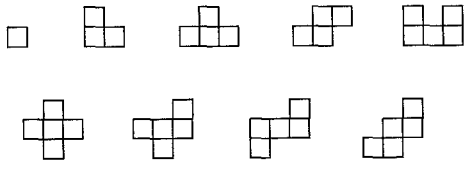

Fig. 8. List of canonical animals of Fig. 1

Now we can define an invariant of an animal A which gives an indication of how complicated its shape is: The *complexity number* of an animal A, with respect to shape, is the number n° of cells in A°.

Each maximal submesh is visible from any one of its interior points. Since squashing of an animal A preserves the number of maximal submeshes, there exist relations between the seeing graphs of animals and that of their canonical forms, as well as a dependence of seeing graphs on the complexity number. These relations will be explored in a subsequent study.

4. Comments and suggestions for future applications

This formulation enables one to use just one positive integer to serve both intuitively and meaningfully as a numerical specification of the complexity of the shape of an animal. Furthermore, every Jordan curve J can be successively approximated by the perimeters of a sequence of square-cell animals of gradually decreasing cell size. Thus, this approach shows promise for leading to a formulation of the complexity of the shape of a curve J.

The approach proposed is also suitable for analyzing shape similarity, illustrating the similarity principle suggested in [9]: geometrical similarity can be treated as topological equivalence. Shape similarity of square-cell animals is defined as an equivalence relation, based on sharing a common canonical form.

Among applications in the natural sciences, the shape characterization of two-dimensional solids and molecular aggregates on the surfaces of catalysts appears to have special importance (see, e.g. [10] and references therein). The complexity measure is expected to show close relations with reactivity, since it is

Table 1. The numbers a_n of animals and c_n of canonical animals for $n \leqslant 5$

n	1	2	3	4	5
a_n	1	1	2	5	12
c_n	1	0	1	2	5

assumed that a two-dimensional cluster of a more "rugged" appearance is likely to undergo both physical rearrangements and chemical reactions more readily than aggregates with smoother boundaries. This "ruggedness" can be characterized using the shape complexity measure proposed in this study. The aggregate itself may also serve as a catalyst, and the solid may take the role of mere support for the two-dimensional aggregate. It is expected that an aggregate with a greater complexity number has a more pronounced catalytic effect.

We plan to investigate later the corresponding development of the complexity of three-dimensional polycubes. These are to two-dimensional surfaces and their shapes as animals are to Jordan curves and their shapes.

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References

1. Harary, F Palmer EM (1973) Graphical Enumeration. Academic Press, New York
2. Soteros C, Whittington SG (1988) J Phys *A* 21:2187
3. Madras N, Soteros C, Whittington SG (1988) J Phys A 21:4617
4. Harary F, Mezey PG (1988) J Math Chem 2:377
5. Harary F, Lewinter M (1988) Int J Computer Math 25:1
6. Harary F (1969) Graph Theory. Addison-Wesley, Reading, Mass
7. Exoo G, Harary F (1987) Nat Acad Sci Lett 10:67
8. Harary F, Mezey PG (1991) Chiral and Achiral Square-Cell Configurations and the Degree of Chirality. In: Mezey PG (ed) New Developments in Molecular Chirality. Kluwer, Dordrecht
9. Mezey PG (1990) Three-dimensional Topological Aspects of Molecular Similarity. In Maggiora GM, Johnson MA (eds) Concepts and Applications of Molecular Similarity. Wiley, New York
10. Silverberg M, Ben-Shaul A (1987) J Chem Phys 87:3178