Monatshefte für Chemie 116, 211—216 (1985)

Monatshefte für Chemie
Chemical Monthly

Note on the Topological Information Content of Simple Graphs*

Oskar E. Polansky

Max-Planck-Institut für Strahlenchemie, D-4330 Mülheim an der Ruhr, Federal Republic of Germany

(Received 17 September 1984. Accepted 1 October 1984)

It is shown that simple graphs gave equal topological information content if their automorphism groups are isomorphic. Further, if the automorphism groups of two graphs are represented by wreath products of which the inner groups are isomorphic, then the two graphs possess equal topological information content. Three graphs which correspond to organic molecules illustrate this finding.

(Keywords: Automorphism groups; Graph theory; Information theory; Topological information content)

Zum topologischen Informationsgehalt einfacher Graphen

Wie gezeigt wird, besitzen schlichte Graphen gleichen topologischen Informationsgehalt, wenn ihre Automorphisgruppen isomorph sind. Ferner: sind die Automorphismengruppen zweier Graphen durch Kranzprodukte darstellbar deren Feingruppen isomorph sind, dann haben diese beiden Graphen gleichen topologischen Informationsgehalt. Drei Graphen, welche mit organischen Molekülen korrespondieren, illustrieren das Ergebnis.

The topological information content, $\bar{I}_{\text{top}}$, of a simple graph, G, (in bits per vertex) is defined[1] as follows:

$$\bar{I}_{\text{top}}(G) = -\sum_{i=1}^{k} (N_i/N) \cdot \text{lb}\,(N_i/N) \qquad (1)$$

where i is the index of the k different subsets V_i of equivalent vertices, $N_i = |V_i|$ their cardinalities, $N = \sum N_i$ the total number of the vertices of G and lb indicates the binary logarithm, i.e. the logarithm to the base 2.

* Dedicated to Professor Dr. *Karl Schlögl* on the occasion of his 60th birthday.

Obviously, $\bar{I}_{top}$ does not depend on the labelling of the vertices of G, therefore, it is an invariant of the graph. We shall show here that, more generally, $\bar{I}_{top}$ is an invariant of several graphs belonging to a class of different automorphism groups, defined by some structural conditions.

At first we shall show that $\bar{I}_{top}$ is an invariant of an automorphism group of given structure. Let $A(G)$ be the automorphism group of the simple graph G. In any automorphism only equivalent vertices may be mapped onto each other. Hence, the structure of $A(G)$ defines the subsets V_i of equivalent vertices and their cardinalities, N_i, too. In that way, obviously $\bar{I}_{top}$ is an invariant of $A(G)$ and consequently the following equation

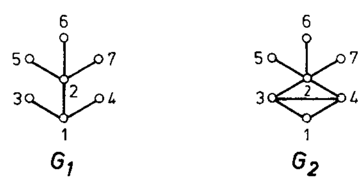
$$\bar{I}_{top}(G_1) = \bar{I}_{top}(G_2) \tag{2a}$$

must hold if the automorphism groups of the two graphs are isomorphic, i.e.:

$$A(G_1) = A(G_2). \tag{2b}$$

As an illustration we present the following example:

Scheme 1



Obviously, G_1 and G_2 are not isomorphic. Both graphs consist of the same total number of vertices, $N = 7$; this is necessary, since as a consequence of the isomorphism of the automorphism groups of the two graphs, eq. (2 b), the degree of the two groups, i.e. the total number of the vertices in G_1 and G_2, respectively, must be the same.

Now, we will verify the validity of eq. (2 b) in the case of our example. We have labelled the vertices of G_1 and G_2 in such a manner, that the subsets $V_i \in G_j$, $j = 1, 2$, are formally the same, namely

$$\begin{aligned} V_1 &= \{1\}, & V_2 &= \{2\}, \\ V_3 &= \{3, 4\}, & V_4 &= \{5, 6, 7\}. \end{aligned} \tag{3}$$

Consequently, the permutations forming $A(G_1)$ and $A(G_2)$, respectively, are formally also the same; they may be constructed by the combination of exactly one permutation of each of the following sets:

$$V_1: \begin{pmatrix}1\\1\end{pmatrix}; \quad V_2: \begin{pmatrix}2\\2\end{pmatrix};$$
$$V_3: \begin{pmatrix}3 & 4\\3 & 4\end{pmatrix}, \begin{pmatrix}3 & 4\\4 & 3\end{pmatrix}; \tag{4}$$
$$V_4: \begin{pmatrix}5 & 6 & 7\\5 & 6 & 7\end{pmatrix}, \begin{pmatrix}5 & 6 & 7\\6 & 7 & 5\end{pmatrix}, \begin{pmatrix}5 & 6 & 7\\7 & 5 & 6\end{pmatrix}, \begin{pmatrix}5 & 6 & 7\\5 & 7 & 6\end{pmatrix}, \begin{pmatrix}5 & 6 & 7\\7 & 6 & 5\end{pmatrix}, \begin{pmatrix}5 & 6 & 7\\6 & 5 & 7\end{pmatrix}.$$

This mode of construction leads to the following order of $A(G_j)$

$$h(A(G_j)) = 1.1.2.6 = 12. \tag{5}$$

The permutations, denoted in eq. (4), reflect that the identical group operates on the subsets V_1 and V_2, the symmetric group S_2 on the subset V_3, and the symmetric group S_3 on the subset V_4. Hence, $A(G_j)$ may be expressed as a direct product of these groups (E_2 denotes the identical group of degree 2, operating on $V_1 \cup V_2$) as follows:

$$A(G_1) = A(G_2) = E_2 \times S_2 \times S_3 \tag{6}$$

Again, the order of $A(G_j)$ is as follows

$$h(A(G_j)) = h(E_2) \times h(S_2) \times h(S_3) = 1 \times (2!) \times (3!) = 12;$$

and for the degree of $A(G_j)$ one obtains

$$d(A(G_j)) = d(E_2) + d(S_2) + d(S_3) = 2 + 2 + 3 = 7.$$

(Notice, that $E_1 = S_1$, $E_2 = S_1 \times S_1$, etc.).

Because the vertices of G_1 and G_2 are partitioned into the same number of subsets of equivalent vertices, which have pairwise the same cardinalities, namely

$$N_1 = 1,\ N_2 = 1,\ N_3 = 2,\ N_4 = 3,$$

the topological information content of the graphs G_1 and G_2 and of any other simple graph belonging to the automorphism group denoted by eq. (6) is the same and it amounts to

$$\begin{aligned}\bar{I}_{\text{top}}(G_1) &= \bar{I}_{\text{top}}(G_2) = \bar{I}_{\text{top}}(E_2 \times S_2 \times S_3)\\ &= -\frac{1}{7}\,\text{lb}\,\frac{1}{7} - \frac{1}{7}\,\text{lb}\,\frac{1}{7} - \frac{2}{7}\,\text{lb}\,\frac{2}{7}\,\text{lb}\,\frac{2}{7} - \frac{3}{7}\,\text{lb}\,\frac{3}{7}\\ &= 1{,}842\,371 \text{ [bits per vertex]}.\end{aligned}$$

Now, we will show that $\bar{I}_{\text{top}}$ is also an invariant of a certain class of automorphism groups. For that purpose let B and F be two permutation groups and suppose the wreath product $B[F]$ be isomorphic with an automorphism group, $A(G')$, of a simple graph G':

$$A(G') = B[F] \tag{7}$$

then the innergroup, F, acts as an automorphism group on a certain subgraph, $F_j \in G'$ (if necessary, F may contain some half edges in order to keep vertices nonequivalent when they are non-equivalent in G')[2]. The vertex set of F may be denoted by V^{F_j}; certainly, V^{F_j} is a subset of the vertex set $V(G')$ of the graph G' and its cardinality, N^F, is the degree of the group F: $|V^{F_j}| = N^F = d(F)$. As shown above in the example, the structure of the group F will partition the vertex set V^F into several subsets, V_i^F, $1 \leqq i \leqq k$, of the respective cardinalities N_i^F.

The graph G' contains altogether $d(B)$ subgraphs isomorphic with F_j, where $d(B)$ denotes the degree of the outer group B of the wreath product given by eq. (7). Hence, the cardinality of the vertex set $V(G')$ of the graph G' is given by

$$|V(G')| = |V^F| \cdot d(B) = N^F \cdot d(B) = N. \tag{9 a}$$

As a result of the permutations forming the outer group B the subgraphs F_j, $1 \leqq j \leqq d(B)$, are mapped onto each other. In the course of these automorphic mappings the vertices belonging to $V_i^{F_j}$ can only be mapped onto themselves or onto vertices belonging to the corresponding subset $V_i^{F_j'}$ of another subgraph F_j'. This means, that G' does not contain more subsets of equivalent vertices than F_j does, i.e. the partitioning of $V(G')$ into subsets, $V_i(G')$, $1 \leqq i \leqq k$, of equivalent vertices is induced by the inner group F of the wreath product. The cardinalities of these subsets are given by

$$|V_i(G')| = |V_i^F| \cdot d(B) = N_i^F \cdot d(B) = N_i. \tag{9 b}$$

As seen from eqs. (9 a) and (9 b) the ratios N_i/N appearing in eq. (1) are independent of the outer group B of the wreath product eq. (7); they depend only on the structure of the inner group F; due to

$$N_i/N = N_i^F/N^F. \tag{10}$$

Hence, the information content of two graphs of which one belongs to the automorphism group F and the other one to $B[F]$ are equal each other

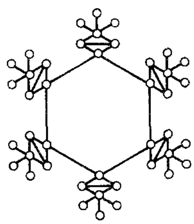
$$\bar{I}_{\text{top}}(F) = \bar{I}_{\text{top}}(B[F]). \tag{11}$$

The structure of B has no influence to that result.

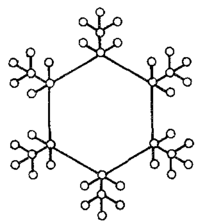
As an illustration we give below G_1' and G_2' constructed from G_1 and G_2

given above, when the outer group B is choosen as the cyclic group C_6 of degree 6:

Scheme 2



G'_1



G'_2

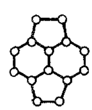
$$A(G'_1) = A(G'_2) = C_6[E_2 \times S_2 \times S_3]. \tag{12}$$

The graphs used above for illustration have no chemical significance. The following three graphs, G_3, G_4, and G_5, represent chemical structures; they possess equal information content, namely

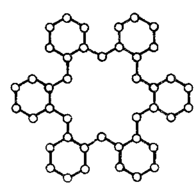
$$\bar{I}_{top}(G_3) = \bar{I}_{top}(G_4) = \bar{I}_{top}(G_5) = 1{,}950212 \text{ [bits/vertex]}.$$

Scheme 3

G_3



G_4



G_5

Obviously, this a consequence of the fact that the automorphism groups of these graphs

$$A(G_3) = E_1 \times S_2[E_3];$$
$$A(G_4) = S_2[E_1 \times S_2[E_3]];$$
$$A(G_5) = C_6[E_1 \times S_2[E_3]].$$

have the factor $[E_1 \times S_2[E_3]]$ in common.

Conclusion

The topological information content of a simple graph, $\bar{I}_{top}$, is not only an invariant of a certain graph but it is a topological characteristic for all graphs which belong either to one and the same automorphism group, F, or to an automorphism group which may be represented by a wreath product where F is the inner group. This result should be considered when the topological information content is used in chemistry.

Acknowledgement

The helpful assistance of Mrs. *R. Wolf, T. Kammann, R. Speckbruck,* and Mr. *H. Gruen* in the preparation of the manuscript is appreciated.

References and Notes

[1] *Bonchev D.,* Information Theoretic Indices for Characterization of Chemical Structures, Chemometric Series (*Bawden D.,* ed.), Vol. 5, p. 83, eq. (77). Chichester: Research Studies Press, J. Wiley. 1983.

[2] If necessary, F may contain some half edges in order to keep vertices nonequivalent when they are nonequivalent in G'. For an illustration see the graph G'' below: the vertices a and b are nonequivalent in G''; without the two half edges at the vertex b in F'' they would become equivalent.

Scheme 4