1090 *J. Chem. Inf. Comput. Sci.* **1994,** *34,* 1090–1093

Rotagraphs and Their Generalizations

Tomaž Pisanski* and Arjana Žitnik

Institute of Mathematics, Physics and Mechanics, Jadranska 19, 61111 Ljubljana, Slovenia

Ante Graovac

The Rugjer Bošković Institute, HR-41001 Zagreb, POB 1016, Croatia

Anton Baumgartner

University of Ljubljana, Department of Mathematics, Jadranska 19, 61111 Ljubljana, Slovenia

Received May 18, 1994®

The chemical concept of polymers can be applied to graph theory in order to define polygraphs. The most useful polygraphs are rotagraphs. They present a concise description of large graphs. By allowing distant monographs to be mutually connected as well as linked to some particular vertices generalizations of rotagraphs are achieved. Generalized rotagraphs appear as a convenient means to describe a series of highly symmetrical polyhedra and fullerene graphs.

INTRODUCTION

Polymers are described graph-theoretically by polygraphs.[1] In a similar way as a polymer is built from monomers, a polygraph is obtained from smaller building blocks, called monographs.

Cycles are frequently used graphs, e.g., in chemistry they represent annulenes. *Cycle* C_m with m vertices is depicted in Figure 1.

Let us replace the vertex set $V(C_m)$ of C_m by a set G_1, G_2, ..., G_m of arbitrary, mutually disjoint graphs. We call them *monographs* in analogy with the chemical notion of monomers. Let us further replace a single edge e_i of C_m by a set of edges, $X_i \subseteq V(G_i) \times V(G_{i+1})$, connecting the ith and $(i + 1)$th monograph. In particular, when $i = m$, one defines $X_m \subseteq V(G_m) \times V(G_1)$. When all edges are replaced in a similar manner a *polygraph*, $\Omega_m = \Omega_m(G_1, G_2, ..., G_m; X_1, X_2, ..., X_m)$ is obtained with $V(\Omega_m) = V(G_1) \cup V(G_2) \cup ... \cup V(G_m)$, $E(\Omega_m) = E(G_1) \cup X_1 \cup E(G_2) \cup X_2 \cup ... \cup E(G_m) \cup X_m$ where $E(G)$ denotes the edge set of G. The name originates from the chemical analogy: in a similar way as a polymer is built from monomers, a polygraph is built from smaller building graphs, call monographs.

Note that Ω_m is closed on itself. A polygraph Γ_m which is open on its ends can be viewed as a special case of $\Omega/_m$ with $X_m = 0$ being an empty set. Γ_m represents a generalization of the path P_m (Figure 1).

ROTAGRAPHS

Further on we assume the uniformity of the monographs and edges connecting them: $G = G_1 = G_2 = ... = G_m$, $X = X_1 = X_2 = ... = X_m$. The appropriate polygraph with closed ends is called a *rotagraph* and denoted by $\omega_m = \omega_m(G;X)$; the polygraph with open ends is called *fasciagraph* and denoted by $\gamma_m = \gamma_m(G;X)$. Results on various graph theoretical invariants of interest in chemistry (the matching[2] and characteristic polynomials,[2,3] perfect matchings,[4] Hosoya index,[5] algebraic structure count,[6] domination number,[7] and others[8]) in rota- and fasciagraphs have been presented in the literature.

® Abstract published in *Advance ACS Abstracts,* September 1, 1994.

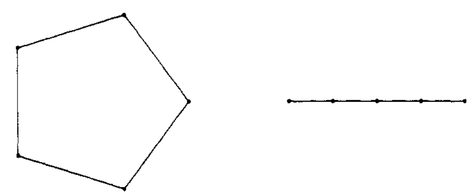


Figure 1. Cycle C_m and path P_m for $m = 5$.

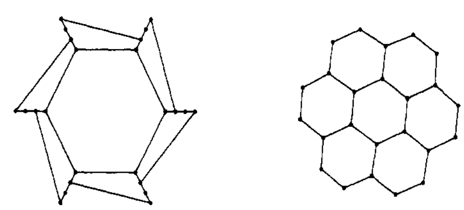


Figure 2. Rotagraph $\omega_6(4;\{\{1,1\},\{4,2\}\})$ with monograph P_4 and its "Nice-Graph" geometrical representation.

Generally, different monographs and connecting edges could lead to the same rotagraph. A very convenient situation arises when the monograph G is a path. In such a case we use a shorthand notation: $\omega_m(P_n;X)$ is abbreviated to $\omega_m(n;X)$.

Example 1. *Let* $n = 4$ *and* $X = \{\{1,1\},\{4,2\}\}$. *Then the rotagraph* $\omega_6 = \omega_6(4;X)$ *is as in Figure 2.*

ω_6 is a generalization of the cycle C_6 which can be geometrically represented by a hexagon. By replacing each vertex of C_6 by a path P_4 drawn as a straight line coming radially out of hexagon and by representing X with the straight lines, one sets the geometrical representation of ω_6 as in Figure 2. Another representation, also shown in Figure 2, is obtained by using the spring embedding algorithm of Kamada and Kawai[9] which is implemented in the system Vega 0.2 as a Mathematica package NiceGraph.[10] It automatically determines the vertex coordinates of a graph. The result will be called the NiceGraph geometrical representation.

Example 2. *Let r be a positive integer and let*

$$X = \{\{1,1\},\{4,2\},\{7,3\},\{9,5\}, ..., \{r^2,(r-1)^2 + 1\}\}$$
$$= \{\{1,1\}\} \cup \bigcup_{k=1}^{r-1} \bigcup_{l=1}^{k} \{\{k^2 + 2l + 1,(k-1)^2 + 2l\}\}$$

Then the rotagraph $\omega_6(r^2;X)$ *represents coronenoid molecule*

0095-2338/94/1634-1090$04.50/0 © 1994 American Chemical Society

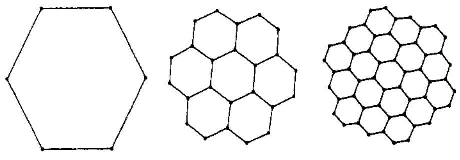


Figure 3. Coronenoid graphs with $r = 1$–3.

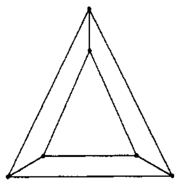


Figure 4. Rotagraph $\omega_3(2;\{\{1,1\},\{2,2\}\})$ represents triangular prism.

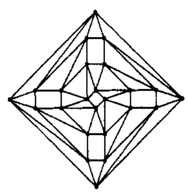


Figure 5. Rotagraph $\omega_4(C_6 + \{\{2,6\},\{3,5\}\};\{\{1,1\},\{1,2\},\{6,2\},\{6,3\},\{5,3\},\{5,4\},\{4,4\}\})$ represents the snub cube.

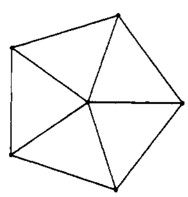


Figure 6. Pyramid graph W_5.

with $6r^2$ carbon atoms. Coronenoid graphs with $r = 1$–3 are shown in Figure 3.

We would like to point out that the example 2 is representative of the coronene one-isomer series first presented by Dias.[17,18]

Example 3. *Let $n = 2$ and let $X = \{\{1,1\},\{2,2\}\}$. Then the rotagraph $\omega_m(n;X)$ represents the graph of m-sided prism. The case $m = 3$ is shown in Figure 4.*

Example 4. *Let*

$$X = \{\{1,1\},\{1,2\},\{6,2\},\{6,3\},\{5,3\},\{5,4\},\{4,4\}\}$$

and let G be a graph, obtained from C_6 by adding the edges $\{2,6\}$ and $\{3,5\}$. Then the rotagraph $\omega_4(G;X)$ in Figure 5 represents the graph of the snub cube. For the definition of snub cube see ref 12.

PYRAMIGRAPHS

Let us connect all vertices of a cycle C_m to an additional vertex u. A graph W_m obtained in the following way

$$V(W_m) = V(C_m) \bigcup \{u\}$$

$$E(W_m) = E(C_m) \bigcup \bigcup_{k=1}^{m} \{k,u\}$$

is depicted in Figure 6. It is called a *wheel* or a *pyramid*; the latter name stems from its geometrical representation.

In a similar way as a cycle was generalized to yield a rotagraph, a pyramid graph can be generalized too: each vertex and edge of C_m is replaced by G and X, respectively, and the distinguished vertex u of W_m is connected by edges

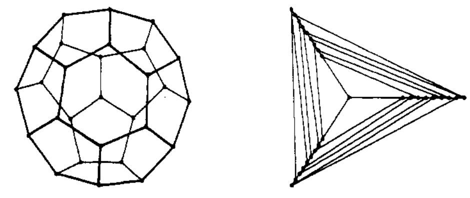


Figure 7. Fullerene C_{28} as a proper pyramigraph $\pi_3(9;\{\{1,3\},\{2,6\},\{4,7\},\{5,9\},\{8,9\}\})$.

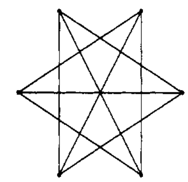


Figure 8. Circulant graph $C(6;2,3)$ is isomorphic to the prism $\omega_3(2;\{\{1,1\},\{2,2\}\})$.

with some subset $Q \subseteq V(G)$ in each copy of G. A graph π_m obtained in such a way

$$V(\pi_m) = V(\omega_m) \bigcup \{u\}$$

$$E(\pi_m) = E(\omega_m) \bigcup \bigcup_{k=1}^{m} \{\{q,u\} | q \in Q_k \subseteq V(G_k)\}$$

where $G = G_1 = G_2 = ... = G_m$, $Q = Q_1 = Q_2 = ... = Q_m$ is called a *pyramigraph*.

A very convenient situation appears when Q contains a single vertex. Such a graph π_m is then called *a proper pyramigraph*. It is denoted by $\pi_m(G;X)$. Proper pyramigraphs with monograph G being a path are of special interest.

Example 5. *Let $G = P_9$ with $X = \{\{1,3\},\{2,6\},\{4,7\},\{5,9\},\{8,9\}\}$ and $Q = \{1\}$. Then the proper pyramigraph π_3 is as in Figure 7. It represents the C_{28} cage (of T_d symmetry) which is the smallest fullerene up to now to form in substantial abundance.*[13]

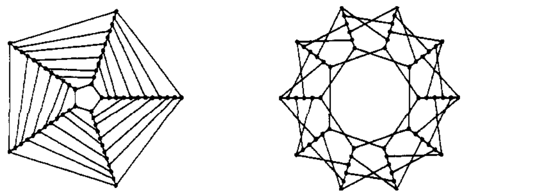
The concept of the pyramigraph can be further generalized by adding the second distinguished vertex and thus obtaining *bipyramigraphs* and in general *polypyramigraphs*.

POLYCIRCULANT GRAPHS

Let us consider a union $v_0 \cup v_1 \cup ... \cup v_{m-1}$ of m disjoint vertices. Let us now connect the vertex v_0 with k distinct vertices $v_{s_1}, v_{s_2}, ..., v_{s_k}$, the vertex v_1 with k distinct vertices $v_{s_1+1}, v_{s_2+1}, ..., v_{s_k+1}$, etc., where s_j's are integers, $1 \leq s_1 \leq s_2 \leq ... \leq s_k \leq (m-1)$. A graph obtained in such a way is denoted by $C(m; s_1, s_2, ..., s_k)$ and is called the *circulant graph*. For consistency we take $v_j = v_{j+m}$, $j = 0, 1, ..., m-1$.

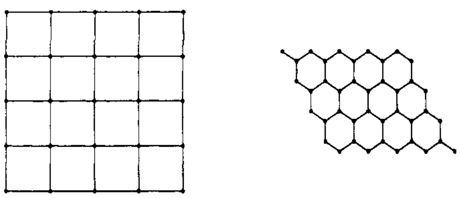
Example 6. *Let* $m = 6$, $k = 2$, $s_1 = 2$, and $s_2 = 3$. *Then the circulant graph $C(6;2,3)$ is as in Figure 8.*

The cycle graph C_n is a special case of the circulant graph $C_n = C(n;1)$. In parallel with generalization of the cycle graphs to rotagraphs, the circulant graphs can be generalized as well by replacing the vertex set of a circulant graph with arbitrary graphs and by replacing every edge of the circulant graph by a set of edges. These generalized graphs are called *polycirculants*. In the special case, where each vertex of the circulant graph $C(m; s_1, ..., s_k)$ is replaced by the same graph G and every edge $\{v_i, v_{s_j+i}\}$ corresponds to the same edge set X_{s_j}, the polycirculant graph is called *the generalized rotagraph*, and it is denoted by $\omega_m(G;X'_{s_1} \cup ... \cup X'_{s_k})$. Here X'_i denotes a set of triples obtained from X_i by adding the index i to each element of X_i, and $X'_1 = X_1$.



(a) (b)

Figure 9. The representation of the I_h:C_{60} fullerene graph (a) as a rotagraph and (b) as a polycirculant $\omega_{10}(6;\{\{1,1,2\},\{3,6\},\{5,4\},\{6,2\}\})$.



(a) (b)

Figure 10. $\omega(1;\{\{1,1\}\},\{\{1,1\}\})$ and $\omega(2;\{\{1,2\}\},\{\{1,2\}\})$.

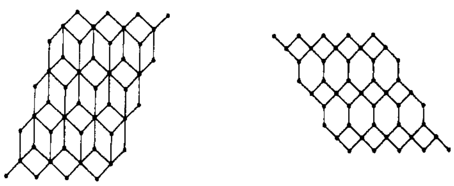


Figure 11. $\omega(3;\{\{2,1\},\{3,2\}\},\{\{2,1\},\{3,2\}\})$ and $\omega(3,\{\{1,2\},\{2,3\}\},\{\{3,1\}\})$.

The procedure is illustrated in Figure 9 where the well-known buckminsterfullerene graph, the I_h:C_{60} fullerene graph, is depicted as a rotagraph (a) as well as a polycirculant (b). The advantage of representing rotagraphs as polycirculants is obvious. The monograph has a smaller number of vertices, and therefore the code is more compact. Moreover, the factorization of various graph-theoretical quantities in rotagraphs becomes simpler, thus enabling their easier computation. For instance, by using this approach, Hosoya was able to obtain the spectrum of I_h:C_{60} graph analytically.[11]

ROTA-ROTAGRAPHS

Allowing monographs to connect in two or more directions, we generalize rotagraphs to *rota-rotagraphs*. The n-dimensional rota-rotagraph can be defined recursively from rotagraphs

$$\omega_{m_1,m_2}(G;X_1,X_2) = \omega_{m_2}(\omega_{m1}(G;X_1), m_1X_2)$$

where m_1X_2 means m_1 times the edge set X_2, each copy going from a distant monograph G, and

$$\omega_{m_1,m_2,\dots,m_n}(G;X_1,X_2,\dots,X_n)$$

$$= \omega_{m_n}(\omega_{m_1,m_2,\dots,m_{n-1}}(G;X_1,X_2,\dots,X_{n-1}),m_1m_2\dots m_{n-1}X_n)$$

Similarly as in one dimension, some ends may be open, and we obtain *fascia-rotagraphs* or, if all the end are open, *fascia-fasciagraphs*. In two dimensions, we can imagine a rota-rotagraph being a torus, fascia-rotagraph being a cylinder, and a fascia-fasciagraph being a part of the plane. Very important are also rota-rotagraphs which are infinite in one or more dimensions. If they are infinite in all dimensions, we omit the indices m_i.

Figures 10–14 show some infinite graphs which can be represented as rota-rotagraphs (graphs from Figures 10–13 are taken from ref 14).

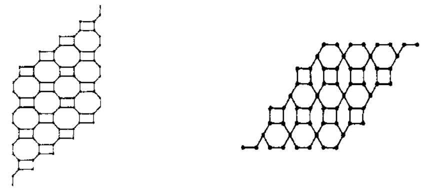


Figure 12. $\omega(4;\{\{3,1\},\{4,2\}\},\{\{4,1\}\})$ and $\omega(5;\{\{1,3\},\{3,5\}\},\{\{1,4\},\{2,5\}\})$.

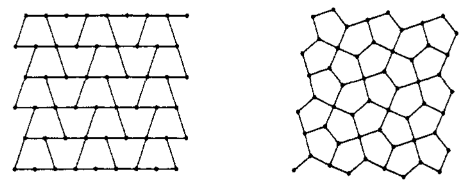


Figure 13. Two drawings of $\omega(P_6 + \{1,5\};\{\{1,3\},\{6,4\}\},\{\{4,2\},\{6,1\}\})$.

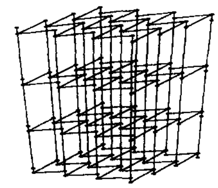


Figure 14. $\omega(2;\{\{1,2\}\},\{\{1,2\}\},\{\{1,2\}\})$.

Example 7. *The most familiar example of a two-dimensional system of indefinite extent is a layer of graphite. It can be represented as* $\omega(2;\{\{1,2\}\},\{\{1,2\}\})$, *as in Figure 10b.*

Example 8. *Three-dimensional rota-rotagraphs can be applied to represent crystals. The topology of an infinite diamond crystal can be represented as* $\omega(2;\{\{1,2\}\},\{\{1,2\}\},\{\{1,2\}\})$, *see Figure 14.*

CONCLUSION

Rotagraphs and rota-rotagraphs are not new. They are known mathematical objects. They are a special case of *covering graphs*. See for instance ref 15. Rotagraphs are exactly those covering graphs that can be described with voltage graphs whose voltage group is cyclic, and the voltages are either 0 or 1. The rota-rotagraphs have Abelian voltage group. Finally, the polycirculant graphs are exactly the covering graphs with cyclic voltage group. Some of these facts are mentioned and developed in the diploma thesis.[16]

ACKNOWLEDGMENT

This work was supported in part by the Ministry of Science and Technology of Slovenia under the Grant 51-0010-0101-94. One of us (A.G.) gratefully acknowledges partial financial support from the Open Society-Croatia Foundation. He would also like to thank the Deutscher Akademischer Austauschdienst for a Fellowship and Prof. K. Schaffner, Dr. F. Mark, and Dr. V. Bachler for the friendly and stimulating atmosphere provided during his stay (September-October'93) at the Max-Planck-Institut für Strahlenchemie, Mülheim/Ruhr, Germany.

REFERENCES AND NOTES

(1) Polansky, O. E.; Tyutyulkov, N. N. Structural Graphs of Regular Polymers and Their Properties. *MATCH* **1977**, *3*, 149–223.
(2) Babić, D.; Graovac; A.; Mohar, B.; Pisanski, T. The Matching Polynomial of a Polygraph. *Discr. Appl. Math.* **1986**, *15*, 11–24.
(3) Graovac, A.; Polansky, O. E.; Tyutyulkov, N. N. Acyclic and Characteristic Polynomial of Regular Conjugated Polymers and Their Derivatives. *Croat. Chem. Acta* **1983**, *56*, 325–356.
(4) Graovac, A.; Babić, D.; Strunje, M. Enumeration of Kékule Structures in Polymers. *Chem. Phys. Lett.* **1986**, *123*, 433–436.

(5) Gutman, I.; Kolaković, N.; Graovac, A.; Babić, D. A. Method for Calculation of the Hosoya Index of Polymers. *Studies Phys. Theor. Chem.* **1989**, *63*, 141–154.
(6) Gutman, I. Algebraic Structure Count of Linear Phenylenes. *Indian J. Chem.* **1993**, *32A*, 281–284.
(7) Klavžar, S.; Žerovnik, J. Algorithmic Approach to Fasciagraphs and Rotagraphs. *Prepr. Series, Univ. Ljubljana, Institute Math. Phys. Mech. Ljubljana, Slovenia* **1994**, *32*, No. 436, 1–11.
(8) Seitz, W. A.; Klein, D. J.; Graovac, A. Transfer Matrix Methods for Regular Polymer Graphs. *Studies Phys. and Theor. Chem.* **1988**, *54*, 157–171.
(9) Kamada, T.; Kawai, S. An Algorithm for Drawing General Undirected Graphs. *Inform. Process. Lett.* **1989**, *31*, 7–15.
(10) Pisanski, T.; Graovac, A. Manuscript in preparation.
(11) Hosoya, H.; Tsukama, Y. Efficient Way for Factorizing the Characteristic Polynomial of Highly Symmetrical Graphs such as Buckminsterfullerene. *Full. Sci. Technol.* In press.
(12) Cundy, H. M. *Mathematical Models*, 3rd. ed.; Tarquin Publications: Stradbroke Diss Norfolk, 1981.
(13) Guo, Ting; et al. Uranium stabilization of C_{28}: a tetravalent fullerene. *Science* **1992**, *257*, 1661–1664.
(14) Sachs, H. in *Topics in Combinatorics and Graph Theory*. Physica-Verlag: Heidelberg, 1990; pp 577–584.
(15) Gross, J. T.; Tucker, T. W. *Topological Graph Theory*; Wiley Interscience: 1987.
(16) Baumgartner, T. *Rotagraphs*, (Slovenian) Ljubljana, 1994. Odd. za matematiko, University of Ljubljana.
(17) Dias, J. R. A periodic Table for Polycyclic Aromatic Hydrocarbons. Isomer Enumeration of Fused Polycyclic Aromatic Hydrocarbons. 1. *J. Chem. Inf. Comput. Sci.* **1982**, *22*, 15–22.
(18) Dias, J. R. Benzenoid Series Having a Constant Number of Isomers. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 61–64.