Revue Roumaine de Chimie, **33**, 7, 709—717 (1988)

CHEMICAL GRAPH POLYNOMIALS. 1

THE POLYNOMIAL DESCRIPTION OF GENERALIZED CHEMICAL GRAPHS

OVIDIU IVANCIUC *
Polytechnic Institute "Traian Vuia", Faculty of Chemical Technology, Timişoara, Romania

Received May 16, 1987

An alternative formulation of the Sachs formula which relates the structure of a generalized graph and its μ, and acyclic ploynomials is given. Some recurrence rèlations for the generalized μ, characteristic and acyclic polynomials are presented.

1. INTRODUCTION

The graph theoretical polynomials [1] play a significant role in the area of topological chemistry, with applications to diverse areas such as the topological resonance theory (TRE) [2,3] and the topological effect on molecular orbitals (TEMO).[4] The most used graph theoretical polynomials are the characteristic, the acyclic (matching) and the μ-polynomial. We will present a slightly different formulation of the Sachs formula applied to generalized graphs. Some expressions for the generalized μ, characteristic and acyclic polynomials are obtained.

2. NOTATION AND TERMINOLOGY

We shall use the standard graph notation and terminology. G will denote a graph with n vertices : $v_1, v_2, \ldots, v_n$, m edges and r cycles : $C_1, C_2, \ldots, C_r$. We denote by t_i the weight associated to the cycle C_i. The edge connecting the vertices v_i and v_j is denoted by e_{ij}. The subgraph $G-v_i$ is obtained from the graph G by deletion of the vertex v_i. The subgraph $G-e_{ij}$ is obtained from the graph G by deletion of the edge e_{ij}. The subgraph $G-C_i$ is obtained from the graph G by deleting all the vertices of the cycle C_i. Two cycles, C_i and C_j, are disjoint if they have no vertex in common. We will denote by g_i the degree (the number of neighbours) of the vertex v_i.

---

* Correspondence address : strada N. Grigorescu, 18/2, 2750 Hunedoara, Romania

The characteristic polynomial of the graph G may be expressed as follows

$$\mathrm{Ch}(G, x) = \det|x\mathbf{I} - \mathbf{A}| = \sum_{n=0}^{N} a_n x^{N-n} \tag{1}$$

where $\mathbf{I}$ is the unit matrix and $\mathbf{A}$ is the adjacency matrix of the graph G.[5]

The coefficients a_n of the characteristic polynomial $\mathrm{Ch}(G, x)$ may be computed without using the unpractical procedure of the expansion of the determinant but from the topology of the molecular graph. Such a procedure was given by Sachs[6] in the following expression:

$$a_n = \sum_{s \in S_n} (-1)^{c(s)} 2^{r(s)} \tag{2}$$

where s is a Sachs graph, S_n is the set of all Sachs graphs with n vertices, $c(s)$ is the total number of components in s, and $r(s)$ is the number of cycles in s. The components of a Sachs graph are combinations of isolated bonds (K_2) and cycles (C_m). Recently the Sachs formula was extended to vertex-weighted graphs[7,8] and to vertex- and edge-weighted graphs[9,10], that is to say to those graphs which may be used to represent heteroconjugated molecules.

Hosoya defined[11] the acyclic (matching) polynomial as:

$$\mathrm{Ac}(G, x) = \sum_{k=0}^{N} [(-1)^k P(G, k) x^{N-2k}] \tag{3}$$

where $P(G, k)$ is the number of ways of choosing k disjoint edges from G.

From the two definitions one could hardly anticipate any connection between $\mathrm{Ch}(G, x)$ and $\mathrm{Ac}(G, x)$. This connection is done by the μ-polynomial, $\mu(G, t, x)$, which continuously transforms $\mathrm{Ac}(G, x)$ into $\mathrm{Ch}(G, x)$ when the parameter t changes from zero to unity. Gutman and Polansky defined[12] the μ-polynominal as

$$\mu(G, t, x) = \sum_{n=0}^{N} \sum_{s \in S_n} (-1)^{c(s)} 2^{r(s)} x^{N-n} T(s) \tag{4}$$

where $T(s)$ is the product of the individual weights of the $r(s)$ cycles of the Sachs graphs s.

3. THE GENERALIZED GRAPH AND POLYNOMIALS

The generalized (vertex- and edge-weighted)[10] graph G_g is a graph which has the loop l_i, located at the vertex v_i, weighted with the quantity a_i and the edge e_{ij} weighted with the quantity b_{ij}. We define the generalized set of Sachs graphs as the set formed by loops L, isolated bonds

K_2, and cycles C_m. The contribution of a loop is equal to

$$p(l_i) = a_i \tag{5}$$

that of an weighted edge is equal to

$$p(e_{ij}) = b_{ij}^2 \tag{6}$$

that of an weighted cycle is equal to

$$p(c_i) = \prod b_{ij} \tag{7}$$

where the multiplication goes over all edges in the cycle, and finally, the contribution of a Sachs graph, $p(s)$, is obtained by the multiplication of the contributions of the components of the Sachs graph:

$$p(s) = \prod_{i=1}^{c(s)} p_i \tag{8}$$

Thus, the generalized μ-polynominal is defined as

$$\mu(G_g(t, x)) = \sum_{n=0}^{N} \sum_{s \in S_n} (-1)^{c(s)} 2^{r(s)} p(s) T(s) \tag{9}$$

From the above formula it follows that the generalized characteristic polynomial is given by

$$\mathrm{Ch}(G_g(x)) = \sum_{n=0}^{N} \sum_{s \in S_n} (-1)^{c(s)} 2^{r(s)} p(s) \tag{10}$$

and the generalized acyclic polynomial has the following expresion

$$\mathrm{Ac}(G_g(x)) = \sum_{n=0}^{N} \sum_{s \in S_n} (-1)^{c(s)} p(s) \tag{11}$$

4. RECURRENCE RELATIONS

If the generalized graph G_g is obtained from the graph G by setting the weight of the vertex v_i equal to a and the weight of the edge e_{ij}, $j = \overline{1, g_i}$ equal to b_{ij}, the following equalities take place:

Proposition 1.

$$\mu(G_g) = \mu(G) - a\mu(G - v_i) -$$
$$- \sum^{g_i} (b_{ij}^2 - 1)\mu(G - v_i - v_j) - 2\sum^{f} (p(C_j) - 1) t_j \mu(G - C_j) \tag{12}$$

$$\mathrm{Ch}(G_g) = \mathrm{Ch}(G) - a\mathrm{Ch}(G - v_i) - \tag{13}$$
$$- \sum^{g_i}(b_{ij}^2 - 1)\,\mathrm{Ch}(G - v_i - v_j) - 2\sum^{f}(p(C_j - 1)(\,\mathrm{Ch}(G - C_j)$$

$$\mathrm{Ac}(G_g) = \mathrm{Ac}(G) - a\mathrm{Ac}(G - v_i) - \sum^{g_i}(b_{ij}^2 - 1)\,\mathrm{Ac}(G - v_i - v_j) \tag{14}$$

The second summation in (12) and (13) goes overall f cycles in G which contain vertex v_i.

From the previously known recurrence relations for $\mu(G)$,[12] $\mathrm{Ch}(G)$ [13] and $\mathrm{Ac}(G)$ [11,14]:

$$\mu(G) = \mu(G - e_{ij}) - \mu(G - v_i - v_j) - 2\sum t_j\mu(G - C_j) \tag{15}$$

$$\mathrm{Ch}(G) = \mathrm{Ch}(G - e_{ij}) - \mathrm{Ch}(G - v_i - v_j) - 2\sum \mathrm{Ch}(G - C_j) \tag{16}$$

$$\mathrm{Ac}(G) = \mathrm{Ac}(G - e_{ij}) - \mathrm{Ac}(G - v_i - v_j) \tag{17}$$

we obtain

Proposition 2.

$$\mu(G_g) = \mu\left(G - \sum_{j=1}^{g_i} e_{ij}\right) - a\mu(G - v_i) - \tag{18}$$
$$- \sum_{j=1}^{g_i} b_{ij}^2\mu(G - v_i - v_j) - 2\sum_{j=1}^{f} p(C_j)t_j\mu(G - C_j)$$

$$\mathrm{Ch}(G_g) = \mathrm{Ch}\left(G - \sum_{j=1}^{g_i} e_{ij}\right) - a\,\mathrm{Ch}(G - v_i) - \tag{19}$$
$$- \sum_{j=1}^{g_i} b_{ij}^2\,\mathrm{Ch}(G - v_i - v_j) - 2\sum_{j=1}^{f} p(C_j)\,\mathrm{Ch}(G - C_j)$$

$$\mathrm{Ac}(G_g) = \mathrm{Ac}\left(G - \sum_{j=1}^{g_i} e_{ij}\right) - a\,\mathrm{Ac}(G - v_i) - \sum_{j=1}^{g_i} b_{ij}^2\,\mathrm{Ac}(G - v_i - v_j) \tag{20}$$

The second summation in (18) and (19) goes over all f cycles in G which contain vertex v_i.

Proposition 3.

If every edge e_{ij}, $j = \overline{1, g_i}$, is a bridge then:

$$\mu(G_g) = \mu\left(G - \sum_{j=1}^{g_i} e_{ij}\right) - a\mu(G - v_i) - \sum_{j=1}^{g_i} b_{ij}^2\mu(G - v_i - v_j) \tag{21}$$

$$\mathrm{Ch}(G_g) = \mathrm{Ch}\left(G - \sum_{j=1}^{g_i} e_{ij}\right) - a\,\mathrm{Ch}(G - v_i) - \sum_{j=1}^{g_i} b_{ij}^2\,\mathrm{Ch}(G - v_i - v_j) \tag{22}$$

$$\mathrm{Ac}(G_g) = \mathrm{Ac}\left(G_g - \sum_{j=1}^{g_i} e_{ij}\right) - a\,\mathrm{Ac}(G - v_i) - \sum_{j=1}^{g_i} b_{ij}^2\,\mathrm{Ac}(G - v_i - v_j) \tag{23}$$

The expansion of the μ-polynomial is given in (24) in terms of the μ-polynomials of its subgraphs, corresponding to the decomposition of the graph G and its vertex v_i [15]

$$\mu(G) = x\mu(G - v_i) - \sum_{j=1}^{g_i} \mu(G - v_i - v_j) - 2\sum_{j=1}^{f} t_j\mu(G - C_j) \tag{24}$$

where the second summation goes over all f cycles which contain vertex v_i. For the generalized graph G_g we obtain

Proposition 4.

$$\mu(G_g) = (x - a)\mu(G - v_i) - \sum_{j=1}^{g_i} b_{ij}^2\mu(G - v_i - v_j) - 2\sum_{j=1}^{f} p(C_j)t_j\mu(G - C_j) \tag{25}$$

$$\mathrm{Ch}(G_g) = (x - a)\,\mathrm{Ch}(G - v_i) - \sum_{j=1}^{g_i} b_{ij}^2\mathrm{Ch}(G - v_i - v_j) - 2\sum_{j=1}^{f} p(C_j)\mathrm{Ch}(G - C_j) \tag{26}$$

$$\mathrm{Ac}(G_g) = (x - a)\,\mathrm{Ac}(G - v_i) - \sum_{j=1}^{g_i} b_{ij}^2\,\mathrm{Ac}(G - v_i - v_j) \tag{27}$$

where the second summation in (25) and (26) goes over all f cycles which contain vertex v_i.

In the following propositions, previously established [12] equalities will be presented for the case of the generalized graph G_g.

Proposition 5.

$$\begin{aligned}\mu(G_g) = {} & \mathrm{Ac}(G_g) - 2\sum p(C_i)t_i\,\mathrm{Ac}(G_g - C_i) + \\ & + 4\sum p(C_i)p(C_j)t_it_j\,\mathrm{Ac}(G_g - C_i - C_j) - \\ & - 8\sum p(C_i)p(C_j)p(C_k)t_it_jt_k\,\mathrm{Ac}(G_g - C_i - C_j - C_k) + \dots\end{aligned} \tag{28}$$

In (28) summation goes over all single, pairs, triplets, etc. of mutually disjoint cycles in G_g. The term corresponding to the summation over s mutually disjoint cycles in G_g is:

$$(-1)^s 2^s \sum \left(\prod_1^s p(C_j)\prod_1^s t_j\,\mathrm{Ac}(G_g - C_1 - C_2 - \dots - C_s)\right)$$

The inversion of this identity yields

Proposition 6.

$$\begin{aligned}\mathrm{Ac}(G_g) = {} & \mu(G_g) + 2\sum p(C_i)t_i\mu(G_g - C_i) + \\ & + 4\sum p(C_i)p(C_j)\,t_it_j\mu(G_g - C_i - C_j) + \\ & + 8\sum p(C_i)p(C_j)p(C_k)t_it_jt_k\mu(G_g - C_i - C_j - C_k) + \dots\end{aligned} \tag{29}$$

In (29) summation goes over all single, pairs, triplets, etc. of mutually disjoint cycles in G_g. The term corresponding to the summation over s mutually disjoint cycles in G_g is :

$$2^s \sum \left(\prod_1^s p(C_j) \prod_1^s t_j \mu(G_g - C_1 - C_2 - \ldots - C_s) \right)$$

We express the μ-polynomial in terms of the characteristic polynomial, thus obtaining

Proposition 7.

$$\begin{aligned} \mu(G_g) &= \mathrm{Ch}(G_g) + 2\sum p(C_i)(1 - t_i)\,\mathrm{Ch}(G_g - C_i) + \\ &+ 4\sum p(C_i)p(C_j)(1 - t_i)(1 - t_j)\,\mathrm{Ch}(G_g - C_i - C_j) + \\ &+ 8\sum p(C_i)p(C_j)p(C_k)(1 - t_i)(1 - t_j)(1 - t_k)\,\mathrm{Ch}(G_g - C_i - C_j - C_k) + \ldots \end{aligned} \tag{30}$$

In (30) summation goes over all single, pairs, triplets, etc. of mutually disjoint cycles in G_g. The term corresponding to the summation over s mutually disjoint cycles in G_g is :

$$2^s \sum \left(\prod_1^s p(C_j) \prod_1^s (1 - t_j)\,\mathrm{Ch}(G_g - C_1 - C_2 - \ldots - C_s) \right)$$

The identity (30) can be inverted leading to

Proposition 8.

$$\begin{aligned} \mathrm{Ch}(G_g) &= \mu(G_g) - 2\sum p(C_i)(1 - t_i)\mu(G_g - C_i) \\ &+ 4\sum p(C_i)p(C_j)(1 - t_i)(1 - t_j)\mu(G_g - C_i - C_j) \\ &- 8\sum p(C_i)\,p(C_j)p(C_k)(1 - t_i)(1 - t_j)(1 - t_k)\mu(G_g - C_i - C_j - C_k) + \ldots \end{aligned} \tag{31}$$

In (31) summation goes over all single, pairs, triplets, etc. of mutually disjoint cycles in G_g. The term corresponding to the summation over s mutually disjoint cycles in G_g is :

$$(-1)^s 2^s \sum \left(\prod_1^s p(C_j) \prod_1^s (1 - t_j)\mu(G_g - C_1 - C_2 - \ldots - C_s) \right)$$

Proposition 9.

For $T = 1$ we obtain from (28)

$$\begin{aligned} \mathrm{Ch}(G_g) &= \mathrm{Ac}(G_g) - 2\sum p(C_i)\,\mathrm{Ac}(G_g - C_i) + \\ &+ 4\sum p(C_i)p(C_j)\,\mathrm{Ac}(G_g - C_i - C_j) - \\ &- 8\sum p(C_i)p(C_j)p(C_k)\,\mathrm{Ac}(G_g - C_i - C_j - C_k) + \ldots \end{aligned} \tag{32}$$

The term corresponding to the summation over s mutually disjoint cycles in G_g is

$$(-1)^s 2^s \sum \left(\prod_1^s p(C_j)\,\mathrm{Ac}(G_g - C_1 - C_2 - \ldots - C_s) \right)$$

Proposition 10.
For $T = 0$ we obtain from (29)

$$\begin{aligned}\mathrm{Ac}(G_g) &= \mathrm{Ch}(G_g) + 2\sum p(C_i)\,\mathrm{Ch}(G_g - C_i) + \\ &+ 4\sum p(C_i)p(C_j)\,\mathrm{Ch}(G_g - C_i - C_j) + \\ &+ 8\sum p(C_i)p(C_j)p(C_k)\,\mathrm{Ch}(G_g - C_i - C_j - C_k) + \ldots\end{aligned} \tag{33}$$

The term corresponding to the summation over s mutually disjoint cycles in G_g is

$$2^s \sum \left(\prod_1^s p(C_j)\,\mathrm{Ch}(G_g - C_1 - C_2 - \ldots - C_s) \right)$$

Proposition 11.
If the graph G_g possesses a single cycle C, then

$$\begin{aligned}\mu(G_g) &= \mathrm{Ac}(G_g) - 2p(C)t\,\mathrm{Ac}(G_g - C)\\ \mu(G_g) &= \mathrm{Ch}(G_g) - 2p(C)(1-t)\,\mathrm{Ch}(G_g - C)\\ \mu(G_g) &= (1-t)\,\mathrm{Ac}(G_g) + t\,\mathrm{Ch}(G_g)\end{aligned} \tag{34}$$

$$\begin{aligned}\mathrm{Ch}(G_g) &= \mu(G_g) - 2p(C)(1-t)\mu(G_g - C)\\ \mathrm{Ch}(G_g) &= \mathrm{Ac}(G_g) - 2p(C)\,\mathrm{Ac}(G_g - C)\\ \mathrm{Ch}(G_g) &= \mathrm{Ac}(G_g)(t-1)/t + \mu(G_g)/t\end{aligned} \tag{35}$$

$$\begin{aligned}\mathrm{Ac}(G_g) &= \mu(G_g) + 2p(C)t\mu(G_g - C)\\ \mathrm{Ac}(G_g) &= \mathrm{Ch}(G_g) + 2p(C)\,\mathrm{Ch}(G_g - C)\\ \mathrm{Ac}(G_g) &= \mathrm{Ch}(G_g)t/(t-1) + \mu(G_g)/(1-t)\end{aligned} \tag{36}$$

If the graph G_g possesses s undisjoint cycles,

$$\begin{aligned}\mu(G_g) &= \mathrm{Ac}(G_g) - 2\sum_1^s p(C_i)t_i\,\mathrm{Ac}(G_g - C_i)\\ \mu(G_g) &= \mathrm{Ch}(G_g) + 2\sum_1^s p(C_i)(1-t_i)\,\mathrm{Ch}(G_g - C_i)\end{aligned} \tag{37}$$

$$\mathrm{Ac}(G_g) = \mu(G_g) + 2 \sum_{1}^{s} p(C_i) t_i \, \mu(G_g - C_i)$$
$$\mathrm{Ac}(G_g) = \mathrm{Ch}(G_g) + 2 \sum_{1}^{s} p(C_i) \, \mathrm{Ch}(G_g - C_i) \tag{38}$$

$$\mathrm{Ch}(G_g) = \mu\gamma(G_g) - 2 \sum_{1}^{s} p(C_i)(1 - t_i)\mu(G_g - C_i)$$
$$\mathrm{Ch}(G_g) = \mathrm{Ac}(G_g) - 2 \sum_{1}^{s} p(C_i) \, \mathrm{Ac}(G_g - C_i) \tag{39}$$

The following recurrence relation for the μ-polynomial was given in [12]:

$$\mu(G \cdot H) = \mu(G)\mu(H - v_2) + \mu(G - v_1)\mu(H) - x\mu(G - v_1)\mu(H - v_2) \tag{40}$$

where v_1 and v_2 are vertices of the graphs G and H, respectively, and $G \cdot H$ represents the graph obtained by identifying v_1 with v_2.

Let the weight of the vertex v_i obtained by identifying v_1 with v_2 be a and the weight of the incident edges e_{ij}, $j = \overline{1, g_i}$ be b_{ij}. We obtain the following

Proposition 12.

$$\begin{aligned} \mu(G_g \cdot H_g) = {} & \mu(G_g)\mu(H_g - v_2) + \\ & + \mu(G_g - v_1)\mu(H_g) - (x + a)\mu(G_g - v_1)\mu(H_g - v_2) - \\ & - \sum_{1}^{g_1} (b_{1j}^2 - 1)\mu(G_g - v_1 - v_j)\mu(H_g - v_2) - \\ & - \sum_{1}^{g_2} (b_{2j}^2 - 1)\mu(G_g - v_1)\mu(H_g - v_2 - v_j) - \\ & - \sum (p(C_j) - 1)t_j\mu(G_g - C_j)\mu(H_g) - \sum (p(C_j) - 1)t_j\mu(G_g)\mu(H_g - C_j) \end{aligned} \tag{41}$$

$$\begin{aligned} \mathrm{Ch}(G_g \cdot H_g) = {} & \mathrm{Ch}(G_g) \, \mathrm{Ch}(H_g - v_2) + \\ & + \mathrm{Ch}(G_g - v_1) \, \mathrm{Ch}(H_g) - (x + a) \, \mathrm{Ch}(G_g - v_1) \, \mathrm{Ch}(H_g - v_2) - \\ & - \sum_{1}^{g_1} (b_{1j}^2 - 1) \, \mathrm{Ch}(G_g - v_1 - v_j) \, \mathrm{Ch}(H_g - v_2) - \\ & - \sum_{1}^{g_2} (b_{2j}^2 - 1) \, \mathrm{Ch}(G_g - v_1) \, \mathrm{Ch}(H_g - v_2 - v_j) - \\ & - \sum (p(C_j) - 1) \, \mathrm{Ch}(G_g - C_j) \, \mathrm{Ch}(H_g) - \sum (p(C_j) - 1) \, \mathrm{Ch}(G_g)\mathrm{Ch}(H_g - C_j) \end{aligned} \tag{42}$$

$$\mathrm{Ac}(G_g \cdot H_g) = \mathrm{Ac}(G_g)\,\mathrm{Ac}(H_g - v_2) +$$

$$+ \mathrm{Ac}(G_g - v_1)\,\mathrm{Ac}(H_g) - (x + a)\,\mathrm{Ac}(G_g - v_1)\,\mathrm{Ac}(H_g - v_2) -$$

$$- \sum_{1}^{g_1} (b_{1j}^2 - 1)\,\mathrm{Ac}(G_g - v_1 - v_j)\,\mathrm{Ac}(H_g - v_2) -$$

$$- \sum_{1}^{g_2} (b_{2j}^2 - 1)\,\mathrm{Ac}(G_g - v_1)\,\mathrm{Ac}(H_g - v_2 - v_j)$$

The third and fourth summation in (41) and (42) goes over all cycles in G_g which contain vertex v_1, and over all cycles in H_g which contain vertex v_2, respectively.

5. CONCLUSIONS

Several combinatorial relations between μ, characteristic and acyclic polynomials were extended to generalized graphs. The method exposed is in principle applicable to the description of heteroconjugated molecules in the framework of the HMO theory.

REFERENCES

1. J. V. Knop and N. Triajstić, *Int. J. Quantum Chem.* : *Quantum Chem. Symp.*, **14**, 503 (1980).
2. I. Gutman, M. Milun and N. Trinajstić, *J. Amer. Chem. Soc.*, **99**, 1692 (1977).
3. J. Aihara, *J. Amer. Chem. Soc.*, **98**, 275 (1976).
4. O. E. Polansky and M. Zander, *J. Mol. Struct.*, **84**, 361 (1982).
5. D. H. Rouvray, in "Chemical Application of Graph Theory", A. T. Balaban, Ed. Academic, London, 1976, p. 175.
6. H. Sachs, *Publ. Math. Debrecen*, **1**, 119 (1963).
7. R. B. Mallion, N. Trinajstić and A. J. Schwenk, *Z. Naturforsch.*, **29**a, 1481 (1974).
8. R. B. Mallion, A. J. Schwenk and N. Trinajstić, *Croat. Chem. Acta*, **46**, 171 (1974).
9. A. Graovac, O. E. Polansky, N. Trinajstić and N. Tyutyulkov, *Z. Naturforsch.*, **30a**, 1696 (1975).
10. N. Trinajstić, "Chemical Graph Theory", vol. I, CRC Press, Boca Raton, 1983, p. 56.
11. H. Hosoya, *Bull. Chem. Soc. Japan*, **44**, 2332 (1971).
12. I. Gutman and O. E. Polansky, *Theoret. Chim. Acta (Berl.)*, **60**, 203 (1981).
13. D. Cvetcović, M. Doob and H. Hachs, "Spectra of Graphs — Theory and Application", Academic Press, New York, 1980.
14. I. Gutman and H. Hosoya, *Theoret. Chim. Acta (Berl.)*, **48**, 279 (1978).
15. O. E. Polansky, *Match*, **18**, 71 (1985).