ON THE EXPANSION OF THE µ-POLYNOMIAL OF A SIMPLE GRAPH PARTITIONED INTO SUBGRAPHS WITH AT LEAST TWO COMPONENTS*

Oskar E. Polansky and Ante Graovac**

Max-Planck-Institut für Strahlenchemie, D-4330 Mülheim a.d. Ruhr

(Received: November 16, 1982)

The polynomials play a significant role in graph theory: the characteristic polynomial $\phi(G)$ and the matching polynomial $\alpha(G)$ of the graph G. Recently, a new graphic polynomial, $\mu(G,t)$, has been introduced [1] which reduces to $\phi(G)$ and $\alpha(G)$ for t=1 and t=0 respectively:

$$\mu(G,1) = \phi(G); \ \mu(G,0) = \alpha(G).$$
 (1)

As shown in [1] the $\mu\text{-polynomial}$ obeys the following recursion formula

$$\mu(G) = \mu(G - e_{ij}) - \mu(G - v_i - v_j) - 2t \sum_{i \in J} \mu(G - Z_{ij}); (\underline{2})$$

$$\{Z_{ij}\}$$

here, e_{ij} and z_{ij} denote, respectively, an edge in G incident with the vertices v_i and v_j , and a cycle which contains the edge e_{ij} ; the summation in (2) is over all those cycles.

In chemistry, connected simple graphs G are used to represent tht topological structure of compounds. In certain problems, one considers G as constructed from two partial graphs, say A and B,

and several edges $\{\{a_{\lambda}b_{\lambda}\}\big|a_{\lambda}\in A$, $b_{\lambda}\in B$, $1\leq \lambda\leq 1\}$ which connect them:

$$G = A U B U \{\{a_{\lambda}b_{\lambda}\} \mid 1 \leq \lambda \leq 1\}.$$

Obviously (A \boldsymbol{U} B) is a spanning subgraph of G, and both A and B are induced subgraphs of G [2]; see also Fig. 1.

In the present note, a formula is derived which expresses $\mu(G,t) \text{ in terms of A, B, and } \{a_{\lambda}b_{\lambda}\}.$

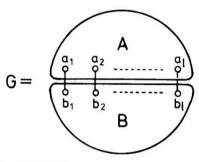


Fig. 1 G as defined by (3).

Before deriving this formula, we will introduce some further notation and confirm some properties of G:

(i) The vertices incident with the edges connecting A and B in G are collected in the subsets $a \in A$ and $b \in B$. From the definition (3) of G, it is obvious that both subsets have equal cardinality, 1:

$$\alpha = \{a_{\lambda} \mid 1 \le \lambda \le 1\},$$

$$b = \{b_{\lambda} \mid 1 \le \lambda \le 1\}.$$

(ii) From the elements of a and b, all the possible subsets are formed (the empty set, ϕ , is such a subset also), denoted by a_o and b_o respectively:

$$\begin{split} & \phi \, \subseteq \, \alpha_{\rho} \, \subseteq \, \alpha \,, \\ & \phi \, \subseteq \, b_{o} \, \subseteq \, b \,. \end{split} \tag{5}$$

Here the index ρ indicates a certain combination of members of the index set $\{\lambda \mid 1 \leq \lambda \leq 1\}$ which is identically the same for a_{ρ} and b_{ρ} . Therefore, the cardinalities of a_{ρ} and b_{ρ} equal each other and obey the relation,

$$0 \le |a_{\rho}| = |b_{\rho}| \le 1.$$

Let $|a_{\rho}| = |b_{\rho}| = r$, there are $\binom{1}{r}$ subsets each of equal cardinality, r; in total there are $L = 2^{1}$ such subsets each. In set theory a system as $\{a_{\rho}\}$ is called the discrete topology of set a.

(iii) The subsets a_{ρ} and b_{ρ} are thought of as being ordered with respect to increasing cardinalities and at constant cardinality, with respect to increasing numbers formed from the indices of ρ as digits. Thus,

(iv) The edges $\{a_{\lambda}b_{\lambda}\}$ will be abbreviated by \bar{a}_{λ} ; the set of all these edges by \bar{a} :

$$\begin{aligned} \overline{a}_{\lambda} &= \{a_{\lambda}b_{\lambda}\} \end{aligned} \tag{\underline{8}}$$

$$\overline{a} &= \{\overline{a}_{\lambda} \mid 1 \leq \lambda \leq 1\} = \{\{a_{\lambda}b_{\lambda}\} \mid 1 \leq \lambda \leq 1\}.$$

Obviously, set \bar{a} is a cutset of G.

(v) Every cycle Z_{ij} appearing in (2) consists of an even number of edges of \bar{a} and the paths connecting them. A cycle which consists of only two edges of \bar{a} , say \bar{a}_{κ} and \bar{a}_{λ} , and the paths $p_{\kappa\lambda}^{A} \in A$ and $p_{\kappa\lambda}^{B} \in B$ leading from a_{κ} to a_{λ} and from b_{κ} to b_{λ} , respectively, is called a simple cycle and, in what follows, such a cycle will be denoted by $\langle \kappa, \lambda \rangle$:

$$\langle \kappa, \lambda \rangle = \bar{a}_{\kappa} U P_{\kappa \lambda}^{A} U \bar{a}_{\lambda} U P_{\kappa \lambda}^{B}$$
 (9)

For the sake of simplicity, from here up to eqn. (29) only the contributions of the simple cycles to the characteristic polynomial of G will be considered. In general there may be more than one path connecting \mathbf{a}_{κ} and \mathbf{a}_{λ} in A, and \mathbf{b}_{κ} and \mathbf{b}_{λ} in B. Since A and B are connected graphs, we have

$$\left| \{ P_{\kappa \lambda}^{A} \} \right| \ge 1 \le \left| \{ P_{\kappa \lambda}^{B} \} \right| \tag{\underline{10}}$$

for each pair κ, λ .

(vi) In forming the set $\{\langle \kappa, \lambda \rangle\}$ of simple cycles, each $P_{\kappa\lambda}^A$ is to combine with each $P_{\kappa\lambda}^B$; hence, one obtains

$$\{ \langle \kappa, \lambda \rangle - \overline{a}_{\kappa} - \overline{a}_{\lambda} \} = \{ P_{\kappa \lambda}^{A} \} (\underline{x}) \{ P_{\kappa \lambda}^{B} \},$$

$$\{ \langle \kappa, \lambda \rangle \} = \{ \{ P_{\kappa \lambda}^{A} \} | \cdot | \{ P_{\kappa \lambda}^{B} \} |.$$

$$(\underline{1}\underline{1})$$

(vii) The superset of all $\{P_{\kappa\lambda}^X\}$, X = A,B, is denoted by ω^X :

$$\omega^{X} = \{\{P_{\kappa\lambda}^{X}\} \mid 1 \leq \kappa \leq \lambda \leq 1\}; \ X = A,B.$$

Obviously the cardinality of w^{X} is given by

$$|\omega^{X}| = \begin{pmatrix} \frac{1}{2} \end{pmatrix} = \omega. \tag{13}$$

(ix) Analogous to (ii), all possible subsets of disjunct paths inclusive of the empty set are constructed from w^X and denoted by w^X_+ :

$$\phi \subseteq = \omega_{\mathsf{T}}^{\mathsf{X}} \subseteq \omega^{\mathsf{X}} \tag{14}$$

these are thought of as being ordered analogous to (iii), so that

As in the case of ρ in (5), (6), and (7), τ represents a certain combination of indices.

Let $\{\omega_{\tau}^X|p=|\omega^X|\}$ be the set of all subsets explained in (ix) which have equal cardinalities, p; obviously, then,

$$p \le \frac{1}{2} \tag{16}$$

It is shown in the Appendix, that the cardinality of the set above is as follows

$$|\{\omega_{\tau}^{X}|p=|\omega_{\tau}^{X}|\}|=[(2p-1)!!]\begin{pmatrix}1\\2p\end{pmatrix}. \qquad (\underline{1}\underline{2})$$

After these preliminaries, we may apply the recursion formula (2) to G removing $\{a_1b_1\}$ and obtain:

$$\mu(G) = \mu(G - \{a_1b_1\}) - \mu(G - a_1 - b_1) - 2t\sum_{\{Z_1\}} \mu(G - Z_1).$$

For the sake of compactness, we introduce the following abbreviations

$$\mu(G) = (G);$$
 $(G - \{a_1b_1\}) = (G - \bar{a}_1),$
 $(G - a_1 - b_1) = (G - a_1);$

in the notation of $\mu\text{-polynomials, }a_{\lambda}$ represents the pair of vertices, formed by a_{λ} and b_{λ} .

Some care is required to evaluate the sum $\sum (G-Z_1)$. First, only the simple cycles will be considered and their contribution to (G) will be indicated by the index s. According to (9) we may rewrite that term as follows:

$$\left[\sum (G-Z_1)\right]_{S} = \sum_{\lambda \neq 1} \sum_{\{<1,\lambda>\}} (G-<1,\lambda>) = \sum (G-<1,\lambda>)$$

where the summation runs over all $\lambda \neq 1$, and for a given λ over the whole sets $\{P_{1\lambda}^A\}$ and $\{P_{1\lambda}^B\}$. With this notation, the equation above reads

$$(G)_{S} = (G-\bar{a}_{1}) - (G-a_{1}) - 2t\sum (G-\langle 1, \lambda \rangle).$$
 $(\underline{18})$

Applying (2) again, and keeping only the contribution of the simple cycles one obtains straightforwardly,

$$\begin{aligned} \left(G\right)_{s} &= \left(G - \overline{a}_{1} - \overline{a}_{2}\right) - \left(G - \overline{a}_{1} - \overline{a}_{2}\right) - 2t\sum_{i}\left(G - \overline{a}_{1} - \langle 2, \lambda \rangle\right) - \\ &- \left(G - a_{1} - \overline{a}_{2}\right) + \left(G - a_{1} - a_{2}\right) + 2t\sum_{i}\left(G - a_{1} - \langle 2, \lambda \rangle\right) - \\ &- 2t\sum_{i}\left[\left(G - \langle 1, \lambda \rangle - \overline{a}_{2}\right) - \left(G - \langle 1, \lambda \rangle - a_{2}\right) - \\ &- 2t\sum_{i}\left[\left(G - \langle 1, \lambda \rangle - \langle 2, \lambda \rangle\right)\right]. \end{aligned}$$

After ordering the terms and taking into account that $\bar{a}_2 \notin (G-\langle 1,2\rangle)$, we obtain for this equation:

$$(G) = (G - \bar{a}_1 - \bar{a}_2) - (G - \bar{a}_1 - a_2) - (G - \bar{a}_1 - a_2) - (G - \bar{a}_1 - \bar{a}_2) + (G - \bar{a}_1 - a_2) - (G - \bar{a}_1 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2) - \sum_{\alpha} (G - \bar{a}_1 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2) - \sum_{\alpha} (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2) + (\underline{19}) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2) - \sum_{\alpha} (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2 - \bar{a}_2) + (G - \bar{a}_1 - \bar{a}_2 - \bar{a}$$

Inspection of (18) and (19) yields:

- (1) Due to the application of (2), each term in (19) refers to a subgraph of G which does not contain the edges removed: sometimes they have been removed without, sometimes together with the incident vertices.
- (2) The right hand side of (19) is a power series in $(-2t)^{\nu}$, $\nu=0,1,2,\ldots$ where ν is exactly the number of independent simple cycles being removed from G. Since the sets of simple cycles which are removed from G may be expressed by the sets ω_{τ}^{X} defined in (ix), it follows immediately that

$$v = |w_{T}| \tag{20}$$

(the superscript X=A,B can be deleted because in the case of simple cycles, both sets, $\omega_{_T}^A$ and $\omega_{_T}^B$ are involved).

(3) The coefficients of $(-2t)^{\nu}$ are sums of μ -polynomials which contribute to the sum with a sign exactly given by $(-1)^{\left|a_{\rho}\right|}$; here, a_{ρ} (as has been explained in (iii)) denotes the set of pairs of vertices, $\{a_{\lambda},b_{\lambda}\}$, which have been removed from G. These sums are complete in a combinatorial sense, i.e. all combinations are taken into account in which no cycles or only simple cycles are involved.

In view of these developments, one obtains the following expression after having applied the recursion formula k times (1 < k < 1) to G:

$$(G)_{\mathbf{k}} = \sum_{\{\omega_{\tau}\}} \sum_{\{\alpha_{\rho}\}} \left\{ (-2t)^{|\omega_{\tau}|} (-1)^{|\alpha_{\rho}|} \cdot (\underline{21}) \right\}$$

$$\cdot (G - \overline{\alpha}(\mathbf{k}, \rho, \tau) - \alpha_{\rho} - \omega_{\tau})$$

Here, the terms have the following meaning:

denotes the set of edges removed from G together with their incident vertices;

$$w_{_{\rm T}}$$
 the set of simple cycles removed from G,
$$w_{_{\rm T}} = \{ <\kappa\,, \lambda> \} \,,$$

$$1 \le \kappa \le k$$
, λ arbitrary;

 $\bar{a}(k,\rho,\tau)$ the set of edges removed from G without their incident vertices.

(22)

This notation is in accordance with (ii), (iii), (iv), (12) and (20). Since in $[G]_k$, the first k edges

$$\{\{a_{\lambda}b_{\lambda}\} | 1 \leq \lambda \leq k\} = \bar{\alpha}(k)$$

are removed from G (alternatively with or without their incident vertices or as an edge of a simple cycle, but each $\tilde{a}_{\lambda} = \{a_{\lambda}b_{\lambda}\}$ can be removed only once, the three sets are related by

$$\begin{split} \overline{a} \left(\mathbf{k}, \rho, \tau \right) &= \overline{a} \left(\mathbf{k} \right) \backslash \overline{a}_{\rho} \backslash [\overline{a} \left(\mathbf{k} \right) \quad \omega_{\tau}]. \end{split} \tag{23}$$

$$\overline{a}_{\rho} \bigwedge [\overline{a} \left(\mathbf{k} \right) \bigwedge \omega_{\tau}] &= \emptyset$$

(The index k in the lefthand side of (21) indicates how often (2)

has been applied; of course the polynomial (G) itself is not a function of k, but the form of the righthand side of (21) does depend on k).

The expression (21) may be verified by means of (18) and (19). For the proof of its validity, we use (21) as starting point for a further application of (2). In order to obtain a synoptical notation, we will use here the following abbreviations:

$$\vec{x} = \vec{a}_{k+1}, \quad x = a_{k+1}$$

Applying (2) to (G), one obtains:

$$(\tilde{G})_{s} = (\tilde{G} - \bar{x})_{s} - (\tilde{G} - x)_{s} - 2t \sum_{s} (\tilde{G} - z_{x})_{s}.$$

It is easily seen that

(a) \bar{x} in $(G-\bar{x})_S$ enlarges the original set $\bar{a}(k,\rho,\tau)$ to $\bar{a}(k+1,\rho,\tau)$ in accordance to (23); therefore one may write:

$$(\widetilde{G} - \overline{x})_{S} = (\widetilde{G} - \overline{\alpha}(k+1, \rho, \tau) - \alpha_{\rho} - \omega_{\tau})_{S} . \tag{24}$$

b) x in $(\widetilde{G}-x)_s$ enlarges a_ρ to a_ρ , $= a_\rho \bigcup \{a_{k+1}\}$. This consequently means $|a_\rho| = |a_\rho| + 1$ and $\overline{a}(k,\rho,\tau) = \overline{a}(k+1,\rho',\tau)$; hence:

$$-(-1)^{\left|\alpha_{\rho}\right|} \cdot (G-x)_{S} = \dots = (-1)^{\left|\alpha_{\rho}\right|} (G-\overline{a}(k+1,\rho',\tau)-a_{\rho},-w_{\tau})_{S} \left(\underline{25}\right)$$

The enlargement of α_{ρ} to α_{ρ} ' also expands the range of one of the summations indicated in (21).

(c)
$$\sum_{G-Z_X} (G-Z_X)_S$$
 denotes $\sum_{G-Z_X} (G-Z_X)_S$

where the summation runs over all $\kappa>(k+1)$ not occuring in ω_{τ} , and for each of these κ 's it runs over the whole sets $\{P_{k+1,\kappa}^{A}\}$

and $\{P_{k+1,\kappa}^B\}$, as discussed earlier in connection with (18). Hence, this term enlarges the original set w_{τ} to w_{τ} , $= w_{\tau} \bigcup \{<\underline{k}+1,\kappa>\}$. Consequently $|w_{\tau}|=|w_{\tau}|+1$ and the range of the other summation indicated in (21) is expanded. Finally from (23), it follows that $\bar{a}(k,\rho,\tau)=\bar{a}(k+1,\rho,\tau')$. Taking these all together, one may write for one of the summands

Since the right hand sides of (24), (25) and (26) have exactly the form of those terms which would be obtained by rewriting (21) for $\lceil (G)_{k+1} \rceil_S$, the validity of Eq. (21) is proved.

Hence, we may use (21) to write down the result of 1 repeated applications of (2) to G:

$$\left[(G) \frac{1}{1}_{\mathbf{S}} = \sum_{\tau} \left\{ (-2\mathsf{t})^{\tau} |w_{\tau}|^{\tau} (-1)^{\tau} |\alpha_{\rho}|^{\tau} \cdot (G-\overline{\alpha}(1,\rho,\tau) - \alpha_{\rho} - w_{\tau})_{\mathbf{S}} \right\}. \qquad (\underline{\underline{22}})$$

Each term in (27) refers to a subgraph of 6 consisting of at least two components, which are induced subgraphs, one of A and the other of B. This means that each term of (27) may be represented by a product of two factors referring to the subgraphs just mentioned. Since the complete edge set $\bar{a}(1)$ belongs neither to A nor to B, its subsets $\bar{a}(1,\rho,\tau)$ appearing in (27) do not play any role in this factorisation. In view of the symmetry expressed in (3), (7), (8) and (15), one obtains immediately:

$$(\mathcal{G} - \overline{\alpha} (1, \rho, \tau) - a_{\rho} - w_{\tau})_{s} = (A - a_{\rho} - w_{\tau}^{A}) (B - b_{\rho} - w_{\tau}^{B})_{s}$$

Substitution of this into (27) yields the following final result:

$$(G)_{s} = \frac{\sum_{\{\omega_{\tau}\}\{a_{0}\}} \{-2t\}^{|\omega_{\tau}|} (-1)^{|a_{\rho}|} (A-a_{\rho}-w_{\tau}^{A}) (B-b_{\rho}-w_{\tau}^{B})_{s} \}. \quad (\underline{2}\underline{9}).$$

For 1=1,2,3 one has $(G)_S=(G)$ since all cycles constructed by the use of edges of the cutset \overline{a} of cardinality $|\overline{a}|\leq 3$ must be simple cycles. But for $1\geq 4$, (G) differs from $(G)_S$ just due to the existence of cycles containing 4 and more edges of \overline{a} which are not considered in (29). It depends on the actual value of 1, whether some combinations of such cycles $(1\geq 8)$ or with simple cycles $(1\geq 6)$ are possible or not.

Obviously, the difference between these cycles and the simple ones is due to the choice of paths in A and B. To illustrate this point, let us consider the cycles which may be formed by the use of 4 edges of the cutset \bar{a} , say \bar{a}_{κ} , \bar{a}_{λ} , \bar{a}_{μ} , and \bar{a}_{ν} . In the case of simple cycles the indices of the paths used, say $P_{\alpha\beta}^{A}$ and $P_{\xi\eta}^{B}$, must coincide, namely $\{\alpha,\beta\}=\{\xi,\eta\}\subset\{\kappa,\lambda,\mu,\nu\}$. Therefore, altogether 6 sets of single simple cycles and 3 sets of pairs of simple cycles may be constructed; their contribution to (G) is considered in (29). But there are 6 further sets of cycles which contribute to the coefficient of (-2t) in (G) and have not been considered in (29); they may be constructed by pairs of paths in A and B, say $P_{\alpha\beta}^{A}$, $P_{\gamma\delta}^{A}$ and $P_{\xi\eta}^{B}$, $P_{\zeta\omega}^{B}$. Obviously the index sets must coincide, i.e. $\{\alpha,\beta,\gamma,\delta\}=\{\xi,\eta,\zeta,\omega\}=\{\kappa,\lambda,\mu,\nu\}$, but in order not to repeat sets of simple cycles the requirement: $\{\alpha,\beta\}\neq\{\xi,\eta\}\neq\{\gamma,\delta\}$ has to be fulfilled.

This consideration may be generalized for any value of 1. A given set of paths, ω_{τ}^{A} , as expressed in (15), defines a subset of the linking edges, $\bar{a}(\omega_{\tau}^{A})\subseteq\bar{a}$, and similarly ω_{σ}^{B} defines $\bar{a}(\omega_{\sigma}^{B})\subseteq\bar{a}$. In order to construct all the cyclic contributions of (G) one has to combine each ω_{τ}^{A} with all ω_{σ}^{B} which obey the side condition $\bar{a}(\omega_{\tau}^{A})=\bar{a}(\omega_{\sigma}^{B})$. The number of cycles originating from ω_{τ}^{A} and ω_{σ}^{B} is not further simply $|\omega_{\tau}|$ but $Z(\omega_{\tau}^{A}, \omega_{\sigma}^{B})$. The actual value of this number is obtained as the number of smallest subsets into which ω_{τ}^{A} and ω_{σ}^{B} may be partitioned according to

$$\omega_{\tau}^{A} = \bigcup_{\{\gamma\}} \omega_{\gamma}^{A}; \qquad \omega_{\sigma}^{B} = \bigcup_{\{\gamma\}} \omega_{\gamma}^{B}; \qquad (\underline{3}\underline{0})$$

 $\bar{a}\,(\omega_{\gamma}^{\rm A})=\bar{a}\,(\omega_{\gamma}^{\rm B}$,) for each γ where the $\omega_{\gamma}^{\rm A}$ and $\omega_{\gamma}^{\rm B}$, are defined by (15). From the side condition $\bar{a}\,(\omega_{\tau}^{\rm A})=\bar{a}\,(\omega_{\sigma}^{\rm B})$, used above and eqn. (23) one further obtains

$$\bar{a}_{o} \cap \bar{a}(\omega_{\tau}^{A}) = \bar{a}_{o} \cap \bar{a}(\omega_{\sigma}^{B}) = \emptyset$$
 . (31)

All these considerations show in which way a final formula for the characteristic polynomial (G) of a graph G may be derived from eqn. (29) where all cyclic contributions are taken into account: one has to replace (i) the summation over $\{w_{\tau}^{}\}$ by summations over $\{w_{\tau}^{A}\}$ and $\{w_{\sigma}^{B}\}$ where $\bar{a}(w_{\sigma}^{B})=\bar{a}(w_{\tau}^{A})$; (ii) the exponent $|w_{\tau}^{}|$ by $Z(w_{\tau}^{A}, w_{\sigma}^{B})$; and (iii) the set w_{τ}^{B} in $(B-b_{\rho}-w_{\tau}^{B})$ by w_{σ}^{B} . According to this one obtains the following final result:

$$(G) = \sum_{\{\omega_{\tau}^{\mathbf{A}}\}} \sum_{\{\omega_{\sigma}^{\mathbf{B}}\}} \sum_{\{\alpha_{\rho}\}} (-2t)^{\mathbf{Z}} (\omega_{\tau}^{\mathbf{A}}, \omega_{\sigma}^{\mathbf{B}}) (-1)^{|\alpha_{\rho}|} (\mathbf{A} - \alpha_{\rho} - \omega_{\tau}^{\mathbf{A}}) (\mathbf{B} - b_{\rho} - \omega_{\sigma}^{\mathbf{B}})$$

$$\bar{\alpha} (\omega_{\sigma}^{\mathbf{B}}) = \bar{\alpha} (\omega_{\tau}^{\mathbf{A}})$$

$$(\underline{3}\underline{2})$$

Equation (32) is of some use in a systematic investigation of topological effects in chemistry [3].

Appendix

Here, Eq. (17)

$$|\{w_{\tau}^{X}|p=|w_{\tau}^{X}|\}| = \frac{1}{2^{p}} \cdot \frac{(2p)!}{p!} \binom{1}{2p} = w(p)$$

is proved:

- (1) Since $|w_{\tau}^X| = p$, there are p disjunct path sets $\{P_{\kappa\lambda}^X\}$ forming w_{τ}^X . This means that τ represents a certain combination of 2p indices, taken from the 1 indices $\{\lambda \mid 1 \leq \lambda \leq 1\}$.
- (2) Obviously, there are exactly $\binom{1}{2p}$ different combinations of 1 elements to the order of 2p. Each one may be realized in several w_{τ}^{X} , because τ indicates not only a certain combination of indices, but, according to (15), it also expresses a certain pairing of the indices. Therefore, w(p) may be written as a product of two factors

$$w(p) = f(2p) \cdot \begin{pmatrix} 1 \\ 2p \end{pmatrix}$$

where f(2p) counts the inequivalent pairings of 2p indices.

(3) Without any loss of generality, we may consider that combination τ, where the indices are 1,2,3,....,2p-1,2p. The index 2p can be paired with each one of the other (2p-1) indices; hence, in f(2p) there is a factor of (2p-1) involving the pairing of the index 2p with the other one. The remaining (2p-2) indices are paired with each other in f(2p-2) different ways. Therefore, we have the recursion formula

$$f(2p) = (2p-1) \cdot f(2p-2)$$
.

Since

$$f(2)=1;$$
 $f(4)=3,$

by complete induction it follows that

$$f(2p) = 1 \cdot 3 \cdot 5 \cdot \dots \cdot (2p-1) = (2p-1)!!$$

(4) Introduction of this into the expression for w(p) yields Eq. (17).

Annotations

- * This paper replaces a paper received on 15.12.1981, accepted for publication in Match, and cited as Ref. 9 in [3]. The replacement takes place because in the meantime some generalization has been achieved.
- **Permanent address: Institute "R. Bosković", 41001 Zagreb, POB 1016, Croatia, Yugoslavia.

References

- [1] I. Gutman and O.E. Polansky,

 Theoret.Chim.Acta [Berlin], 60, 203 (1981)
- [3] O.E. Polansky and M. Zander, J. Mol. Struct. 84, 361 (1982)