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Research Notes on the Topological Effect on Molecular Orbitals (TEMO); 5*.

A Structure Kit for the Generation of Topomers Exhibiting TEMO without Inversions.

J. Kruszewski** and O.E. Polansky

Max-Planck-Institut für Strahlenchemie,
Stiftstrasse 34-36, 4330 Mülheim a. d. Ruhr (Germany)

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A new method for the generation of topomers exhibiting TEMO without inversions, called C-formation, is presented. A kit of structures needed in that procedure is given.

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* For Part 4 see ref. [1].

** Permanent address: University of Gdansk, Institute of Chemistry, Sobieskiego 18, PL-80952 Gdansk/Poland.

1. Introduction

For particular pairs of topologically related isomers (= topomers), S and T, the Topological Effect on MO (TEMO) predicts an interlacing of the MO energies according [2,3] to

$$\ldots x^S_{2k-1} \leqq x^T_{2k-1} \leqq x^T_{2k} \leqq x^S_{2k} \leqq x^S_{2k+1} \leqq x^T_{2k+1} \leqq x^T_{2k+2} \leqq x^S_{2k+2} \ldots, \quad (1)$$

where x^S_κ and x^T_κ are the MO energies of S and T, respectively, and $\kappa = 1,2,\ldots,n$. This interlacing is a consequence [2,3-6] of

$$\Delta(x) = T(x) - S(x) \geqq 0, \quad x \in (-\infty,+\infty) \quad . \qquad (2)$$

Here, $S(x)$ and $T(x)$ are the characteristic polynomials of the graphs corresponding to the topomers S and T, respectively, and $\Delta(x)$ is called the difference polynomial. Evidently, in order to satisfy eq. (2) $\Delta(x)$ must not have any real zero of odd multiplicity. This requirement is met by particular modes for the construction of the topomers; some examples for such topological models are found in [2,3-11].

Since eq. (1) is derived by nothing other than the topologies of the S and T topomers, at the time it was first tried [2] it was an open question whether that purely topological principle would be recognized within physical reality. Fortunately, eq. (1) can be examined experimentally by means of photoelectron (PE) spectra provided Koopmans theorem holds for the topomers considered. Besides some other evidence as UV absorption energies [2,3,8], the inspection of some hundred PE spectra [2,3,8,12] shows that eq. (1) is satisfied with astonishing accuracy.

The strict demand of eq. (2), i.e. that the difference polynomial $\Delta(x)$ has to be non-negative for any value of x, is obtained for only a few particular topological models [2,4-11]. When the characteristic polynomials of a pair of topomers do not satisfy eq. (2), then the sequence of MO as expressed by eq. (1) is inverted within some intervals, namely in those where $\Delta(x) \leqq 0$. Such inversions are topologically induced because the characteristic polynomials of S and T are topological invariants.

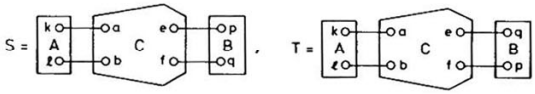
Thus there are two classes of topological models for the formation of topomers: The one class includes all those models for which eq. (2) is obtained while all the other models are collected into the other class.

When the pattern of the PE spectra of a pair of topomers is examined and does not agree with eq. (1), then, in the case that the characteristic polynomials of the topomers also do not satisfy eq. (2), these discrepancies may be either as a consequence of the topology of the topomers or due to physical reasons, such as have been identified in a few particular examples of small molecules by means of SCF calculations and variational perturbation theory [13-15]. In contrast, when the characteristic polynomials of the topomers satisfy eq. (2) but nevertheless the pattern of their PE spectra indicates a deviation from the sequence given by eq. (1) then this can only have a physical cause. Since by use of topological models belonging to the first class, violations of eq. (1) are always due to non-topological reasons, there is some need for further development of models of this class.

The present paper meets that necessity. After a recapitulation of the so-called "model 3" [7,9-11], a procedure called "C-formation" is introduced. By means of this procedure a broad variety of topomers may be generated, the characteristic polynomials of which satisfy eq. (2). A kit of structures useful for C-formation is presented and some examples illustrate its application. Finally, some earlier results are discussed from the new point of view.

2. Model 3

Within this model the topomers S and T are constructed according to the following scheme [11]:



Here we consider only a particular variant of this model characterized as follows:

[M3-1] The terminal moieties are isomorphic, $A \simeq B$, and the vertex $k \in A$ corresponds to $p \in B$ and similarly $\ell \in A$ to $q \in B$.

[M3-2] The central moiety C exhibits a symmetry such that the vertices a and b are equivalent as are also the vertices e and f; i.e., a non-identical automorphic mapping of C comprises the bijections $a \leftrightarrow b$ and $e \leftrightarrow f$.

[M3-3] In order that S and T are connected graphs, at least the vertices a and e and the vertices b and f are connected by disjoint paths; due to [M3-2] these paths have equal lengths.

Under these conditions the difference polynomial takes the following form

$$\Delta = (A^k - A^\ell)^2 (C^{af} - C^{ae}) \tag{3}$$

where $A^k = \phi(A-k,x)$ denotes the characteristic polynomial of the graph obtained from A by removing vertex k, etc.; for details of the concise notations used here see [10].

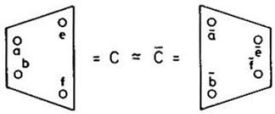
Within this variant of model 3, TEMO without inversions, i.e. a MO sequence according to eq. (1), will result if

$$C^{af} - C^{ae} \geqq 0, \quad x \in (-\infty, +\infty) \ . \tag{4}$$

Thus, the problem of finding structures for S and T satisfying eq. (2) is here reduced to that of finding a central moiety which is in accord with eq. (4). Although some particular examples for such structures of C have already been given [9-11] in the next section a procedure is developed which enables their systematic construction.

3. C-Formation

In order to prepare the induction of the C-formation procedure we have to consider some modes for the partitioning of a given C-moiety. But as a preliminary step we examine two isomorphic C-moieties, $C \simeq \bar{C}$, as shown below:



Because $C \cong \bar{C}$, the two graphs may be isomorphically mapped onto each other. Such a mapping, $C \leftrightarrow \bar{C}$, obviously includes the following bijections:

$$a \leftrightarrow \bar{e}\ , \quad b \leftrightarrow \bar{f}\ , \quad e \leftrightarrow \bar{a}\ , \quad f \leftrightarrow \bar{b}\ ; \tag{5}$$

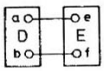
from which it is easily derived that

$$C^{af} - C^{ae} = \bar{C}^{\bar{a}\bar{f}} - \bar{C}^{\bar{a}\bar{e}} \quad . \tag{6}$$

This means: The expression $(C^{af} - C^{ae})$ is invariant under the simultaneous interchange of the vertex labels a with e and b with f. Thus, within model 3 a given C-moiety according to [M3-2], where the vertex pairs $\{a,b\}$ and $\{e,f\}$ are non-equivalent, may be used twice, once in its original form, say C, and then in its $\bar{C}$-form. We call $\bar{C}$ the side-inverted form of C.

We now consider some modes for the partitioning of a given C-moiety into two subunits. From [M3-2] some equalities are derived for the characteristic polynomials of different subgraphs of the subunits; they lead to the cancelling of particular terms in the result obtained by the partitioning.

<u>Mode 1:</u> The following structure of C is assumed:



$$C = D \cup E \cup \{(a,e),(b,f)\} \quad .$$

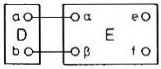
Obviously, the graph corresponding with C^{af} consists of two components; hence, $C^{af} = D^a E^f$ is obtained. The graph corresponding with C^{ae} is connected. The removing of the edge (b,f) leads to $C^{ae} = D^a E^e - D^{ab} E^{ef}$. Thus one has here

$$C^{af} - C^{ae} = D^a E^f - D^a E^e + D^{ab} E^{ef} \quad .$$

As a consequence of [M3-2] $E^f = E^e$; thus the first two terms cancel each other and one obtains finally, in the case of the partitioning mode 1

$$C^{af} - C^{ae} = D^{ab}E^{ef} \quad . \tag{7}$$

Mode 2: Let C have the following structure

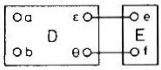


$C = D \cup E \cup \{(a,\alpha),(b,\beta)\}$.

A straightforward calculation, analogous to the above one, leads to

$$C^{af} - C^{ae} = D^{ab}(E^{\alpha f} - E^{\alpha e}) \quad . \tag{8}$$

Mode 3: For the following structure of C



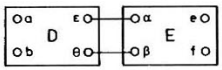
$C = D \cup E \cup \{(\varepsilon,e),(\theta,f)\}$

one obtains

$$C^{af} - C^{ae} = (D^{a\theta} - D^{a\varepsilon})E^{ef} \tag{9}$$

either by a similar straightforward calculation or by applying eq. (6) to eq. (8).

Mode 4: Here, the following structure of C is assumed:



$C = D \cup E \cup \{(\varepsilon,\alpha),(\theta,\beta)\}$.

Removing the edges (ε,α) and (θ,β) from C^{a*}, where the star stands either for e or for f, one obtains

$$C^{a*} = D^{a}E^{*} - D^{a\varepsilon}E^{\alpha*} - D^{a\theta}E^{\beta*} + D^{a\varepsilon\theta}E^{\alpha\beta*} - 2D^{a}_{\varepsilon\theta}E^{*}_{\alpha\beta} \quad .$$

As a consequence of [M3-2] $E^{e} = E^{f}$, $E^{\alpha\beta e} = E^{\alpha\beta f}$, $E^{e}_{\alpha\beta} = E^{f}_{\alpha\beta}$, $E^{\beta e} = E^{\alpha f}$, and $E^{\beta f} = E^{\alpha e}$; hence, the final result can be simplified to

$$C^{af} - C^{ae} = (D^{a\theta} - D^{a\varepsilon})(E^{\alpha f} - E^{\alpha e}) \quad . \tag{10}$$

It is worth noticing that the two factors of the right hand side of eq. (10) are of the same type as the left hand side of eq. (10).

A C-formation is that graph operation which is inverse to the partitioning modes described above and here it will be indicated by the following symbols

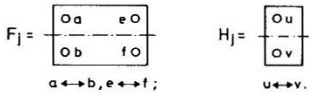
$$C = D \circledast E \quad . \tag{11}$$

This notation may be understood as follows: The graph D is drawn to the left of E. From the crucial vertices of D and E the right hand vertex pair of D is connected with the left hand vertex pair of E by two edges which do not cross each other. From this it is obvious that the graph operation is non-commutative, i.e.

$$D \circledast E \neq E \circledast D \tag{12}$$

provided D and E are non-isomorphic graphs, $D \neq E$, and the vertices $\{a,b\}$ and $\{e,f\}$ are neither equivalent in D nor in E.

This graph operation is only defined upon graphs which belong to special classes $\{F_j\}$ and $\{H_j\}$. Representative members of these classes are given below:



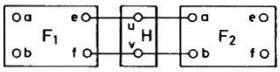
The bijections noted above are required in order to satisfy [M3-2]; they express some symmetry of these graphs which is schematically indicated by the broken line. The four crucial vertices of any F_j are always labelled by a, b, e, and f; those two of H_j by u and v. The graphs used above for C in the partitioning modes 1 - 4 may be expressed as follows: $H_1 \circledast H_2$, $H \circledast F$, $F \circledast H$, and $F_1 \circledast F_2$, respectively; the results obtained for $C^{af} - C^{ae}$ are then as follows: $H_1^{uv} H_2^{uv}$, $H^{uv}(F^{af} - F^{ae})$, $(F^{af} - F^{ae})H^{uv}$, and $(F_1^{af} - F_1^{ae})(F_2^{af} - F_2^{ae})$. It is noteworthy that although the graphs $C_1 = H \circledast F$ and $C_2 = F \circledast H$ are in general non-isomorphic, $C_1 \neq C_2$, they generate the same polynomial

$$(C_1^{af} - C_1^{ae}) = H^{uv}(F^{af} - F^{ae}) = (F^{af} - F^{ae})H^{uv} = (C_2^{af} - C_2^{ae}) \quad . \qquad (13)$$

It is easy to verify that C-formation is an associative graph operation, namely

$$C = (G_1 \circledast G_2) \circledast G_3 = G_1 \circledast (G_2 \circledast G_3) = G_1 \circledast G_2 \circledast G_3 \qquad (14)$$

where G_j, j = 1,2,3 stands for any member of $\{F_j\}$ and/or $\{H_j\}$. This may be illustrated by the following example:



$C = F_1 \circledast H \circledast F_2$,

$$C^{af} - C^{ae} = (F_1^{af} - F_1^{ae})(F_2^{af} - F_2^{ae})H^{uv} \quad . \tag{15}$$

The associative character of the C-formation leads to the following consideration: Suppose a C-moiety is formed from n subunits, namely m F_j and n-m H_j subunits, then one obtains

$$C^{af} - C^{ae} = \prod_{j=1}^{m} (F_j^{af} - F_j^{ae}) \cdot \prod_{j=m+1}^{n} H_j^{uv} \quad . \tag{16}$$

This equality offers the construction of C-moieties from a collection of a few subunits F_j and H_j. Because in eq. (16) $C^{af} - C^{ae}$ is factorized it is relatively easy to select the subunits F_j and H_j so that eq. (4) is satisfied.

It should be noted that from a collection of m F_j and n-m H_j in total $2^{m-1}n!$ non-isomorphic C-moieties can be formed, provided the collection does not include any pair of isomorphic subunits and in all F_j the vertex pairs {a,b} and {e,f} are non-equivalent. According to eq. (16) the polynomials $C^{af} - C^{ae}$ coincide for all these $2^{m-1}n!$ different C-moieties. Clearly the factor n! reproduces the number of different sequences of the F_j and H_j used whilst a factor 2^m arises from the fact that the m subunits F_j may be inserted in a C-moiety either in their original or in their side-inverted forms F_j as explained at the beginning of this section. The collection of these $2^m n!$ C-moieties also includes the side-inverted forms, thus finally $2^{m-1}n!$ non-isomorphic forms result.

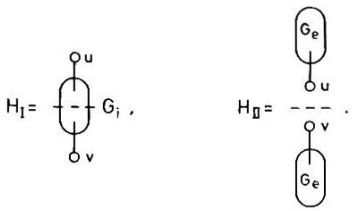
The number $2^{n-1}n!$ increases rapidly with increasing n as may be seen from the first few members of this series:

n	1	2	3	4	5	6	7
$2^{n-1}n!$	1	4	24	192	1 920	23 040	322 560

In practice, however, one will construct C-moieties for topomers which correspond to molecules which are synthesized and the physico chemical properties of which are well investigated; thus, only small values of n will, in general, have relevance.

4. Some Simple Structures for F_j and H_j.

The only requirements which must be satisfied in principle by any graph H_j is that it must consist of at least two vertices and must have a symmetry as expressed by $u \leftrightarrow v$. Thus, one may think of an unlimited number of structures appropriate for H_j. In practice, however, this number will be reduced by the demand that S and T correspond with fully conjugated systems. Then the degree of the vertices u and v in S and T must not exceed the value of 3. Since u and v represent bivalent sites of the subunit H_j they must be univalent in the subunit H_j itself. There are only two types of graphs which agree with all these demands; they are shown below



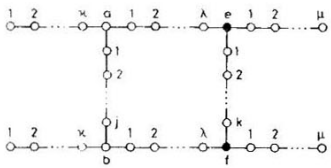
For these types of graphs one obtains

$$H_I^{uv} = G_i \quad ; \tag{17}$$

$$H_{II}^{uv} = G_e^2 \geq 0, \; x \in (-\infty, +\infty) \quad . \tag{18}$$

Since $H_{II}^{uv} \geqq 0$, in regard of eq. (16) a graph of type H_{II} will always agree with the demand of eq. (4). The same is not true in general for graphs of type H_I but is achieved if G_i is either an even-membered Möbius cycle for which $G_i = [\gamma(x)]^2$ holds or the empty graph where $G_i = 1$; in the last case H_I consists only of the two vertices u and v, either connected or disconnected.

The subunits F_j exhibit more variations in their structure as the subunits H_j. A great many of them may be derived from the following quite general graph G_0 by specifying its parameter $\kappa,\lambda,\mu,j,k =$

$G_0 =$ 

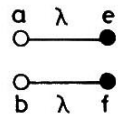
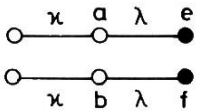
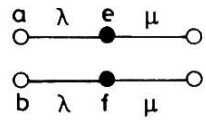
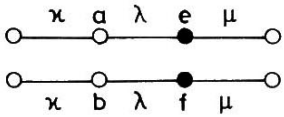
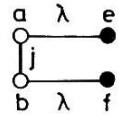
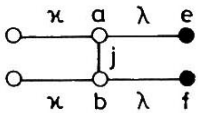
$= 0,1,2,\ldots$. The choice $j = 0$ corresponds with two situations, namely there is either an edge between the vertices a and b or there is no edge between these vertices; the same is true for $k = 0$ and the vertices e and f. Due to [M3-3], however, $\lambda = 0$ always means that the vertices a and e and also b and f are adjacent.

As may be easily verified in the case of G_0 one obtains

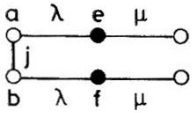
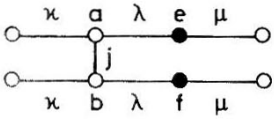
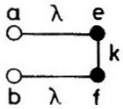
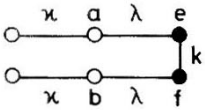
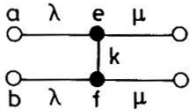
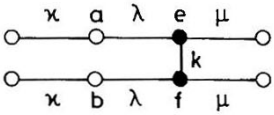
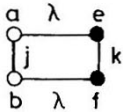
$$G_0^{af} - G_0^{ae} = P_j \, P_k \, P_\kappa^2 \, P_\mu^2 \quad , \tag{19}$$

where $P_j = \phi(P_j,x)$ etc. designates the characteristic polynomial of a path consisting of j vertices. Eq. (19) may be obtained either by a straightforward calculation involving a partitioning of G_0^{af}

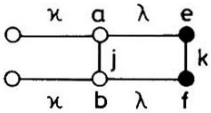
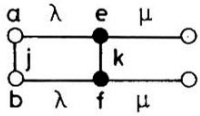
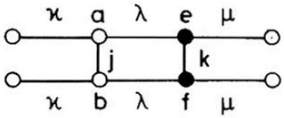
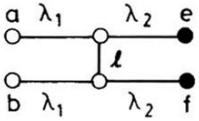
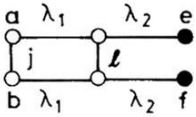
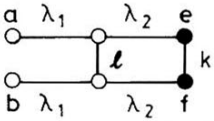
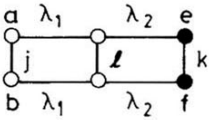
Table 1: Some families of graphs G_τ derived from G_0.

j,	k,	$\varkappa$,	μ,	G_τ		$G_\tau^{af} - G_\tau^{ae}$
0	0	0	0	G_1		1
0	0	-	0	G_2		$P_\varkappa^2$
0	0	0	-	G_3		P_μ^2
0	0	-	-	G_4		$P_\varkappa^2 \; P_\mu^2$
-	0	0	0	G_5		P_j
-	0	-	0	G_6		$P_j \; P_\varkappa^2$

j, k, ϰ, μ, Table 1 (cont.)

- 0 0 -	G_7		$P_j\ P_\mu^2$
- 0 - -	G_8		$P_j\ P_\varkappa^2 P_\mu^2$
0 - 0 0	G_9		P_k
0 - - 0	G_{10}		$P_k\ P_\varkappa^2$
0 - 0 -	G_{11}		$P_k\ P_\mu^2$
0 - - -	G_{12}		$P_k\ P_\varkappa^2 P_\mu^2$
- - 0 0	G_{13}		$P_j\ P_k$

j, k, $\varkappa$, μ, Table 1 (cont.)

- - - 0	G_{14}		$P_j\, P_k\, P_\varkappa^2$
- - 0 -	G_{15}		$P_j\, P_k\, P_\mu^2$
- - - -	G_{16}		$P_j\, P_k\, P_\varkappa^2 P_\mu^2$
	G_{17}		P_ℓ
	G_{18}		$P_j\, P_\ell$
	G_{19}		$P_k\, P_\ell$
	G_{20}		$P_j\, P_k\, P_\ell$

at the vertices b and e and that of G_0^{ae} at the vertices b and f or by means of C-formations using the following subunits: $H_1 = P_{j+2\kappa+2}$, $H_{\lambda+2} = P_{k+2\mu+2}$, and λ subunits H_j, $j = 2,3,\ldots, \lambda + 1$, each one consisting of two vertices only. In this eq. (19) is derived from eq. (16); this illuminates the reason why the result, eq. (19), does not depend on λ, namely, because $H_j^{uv} = 1$ for $j = 2,3,\ldots, \lambda + 1$. As a consequence of this $G_0(j,k,\kappa,\mu)$ represents a particular family of graphs, the members of which are characterized by a distinct value of λ. In the following the term "λ-degeneracy" will refer to that complex of circumstances.

From G_0 several families, G_1 to G_{16}, of subunits may be derived by taking some of the parameters j, k, κ, and μ to be zero. Each family of graphs obtained in this way exhibits λ-degeneracy; they are listed in Table 1. Since $P_0 = 1$, the expressions $G_\tau^{af} - G_\tau^{ae}$, $\tau = 1,2,\ldots,16$ are simply derived from eq. (19). The families G_{17} to G_{20}, also included in Table 1, are obtained by C-formation in accordance with

$$\begin{aligned} G_{17} &= G_9 \circledast G_1 \quad , \\ G_{18} &= G_{13} \circledast G_1 \quad , \\ G_{19} &= G_1 \circledast G_{13} \quad , \\ G_{20} &= G_{13} \circledast G_9 \quad . \end{aligned} \tag{20}$$

Concerning the property

$$\Delta G_\tau \overset{(\underline{\underline{def}})}{=} G_\tau^{af} - G_\tau^{ae} \geqq 0 \quad \text{for all } x \in (-\infty, +\infty)$$

an inspection of Table 1 shows:

(i) $\Delta G_\tau \geqq 0$ holds for $\tau = 1,2,3,4$.

(ii) For $\tau = 5,6,\ldots,12,17$ ΔG_τ consists of some non-negative factors and P_η, $\eta \in \{j,k,\ell\}$; $\Delta G_\tau \geqq 0$ is achieved if $\eta = 0$ is taken.

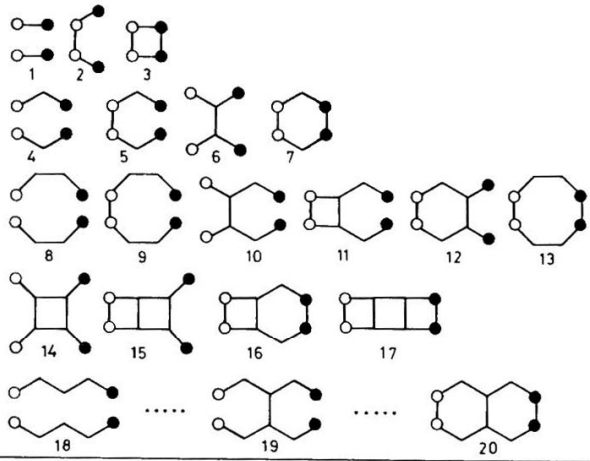
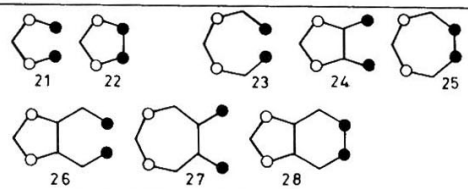
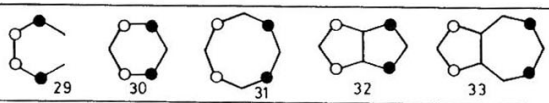
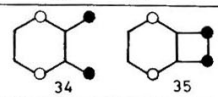
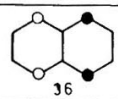
(iii) For $\tau = 13,14,15,16,18,19$ ΔG_τ contains, besides some non-negative factors, the product $P_\eta P_\zeta$, $\eta,\zeta \in \{j,k,\ell\}$; with equal values for the two parameters, $\eta = \zeta = 0,1,2,\ldots$, one arrives at $\Delta G_\tau \geqq 0$.

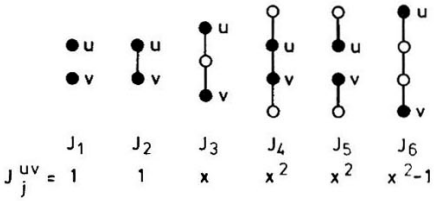
(iv) $\Delta G_{20} = P_j P_k P_\ell$ will be non-negative if two of the three parameters j,k,ℓ equal each other and the third one is zero.

From these families of graphs a series of small subunits F_j may be derived. They are listed in Table 2; this table also contains some further subunits generated by C-formation from the former ones. In all these graphs the vertices a and b are marked by open circles, the vertices e and f by full circles. All these graphs are arranged in Table 2 in such a way that those F_j are grouped together which coincide in their polynomials $\Delta F_j = F_j^{af} - F_j^{ae}$. Since any F_j is isomorphic with its side-inverted form, $\bar{F}_j \simeq F_j$, the latter ones are excluded from the table.

All the subunits F_j given in Table 2 may be generated by C-formation from a few H-type graphs, denoted by J_1 to J_5; they are shown below:

Table 2: A structural kit of subunits F_j for the production of C-moieties within the model 3 by means of C-formation procedure, eq.(16). (By definition: $\Delta F_j = F_j^{af} - F_j^{ae}$)

F_j	ΔF_j
	1
	x
	x^2
	$x^2 - 1$
	$(x^2-1)^2$



The first twenty graphs, 1 to 20, are constructed exclusively from the appropriate numbers of duplicates of J_1 and J_2; thus, according to eq. (16), they all have $\Delta F_j = 1$. For the generation of the subunits 21 to 28 one J_3 and some J_1 and J_2 are used; hence, there a $\Delta F_j = x$ exists. The species 29 accords with $J_2 \circledast J_5$ while the graphs 30 to 33 are made from two J_3 and some J_1 and J_2; hence, in this case $\Delta F_j = x^2$. The subunits 34 and 35 contain one J_6, graph 36 two J_6, hence their ΔF_j are (x^2-1) and $(x^2-1)^2$, respectively.

Table 2 represents a kind of a structural kit for the construction of the central moiety C of model 3 by means of C-formation. In order to generate a C-moiety satisfying eq. (4) one may use an arbitrary number of subunits which have $\Delta F_j \geqq 0$ and/or an even number of subunits which coincide in their ΔF_j. In this way from the kit represented by Table 2 numerous pairs of topomers, S and T, may be constructed which agree with eq. (2); hence, their MO pattern is compatible with eq. (1). Some examples of pairs of topomers produced by means of C-formation using the subunits of Table 2 are collected in Figure 1; they all agree with eqs. (1) and (2).

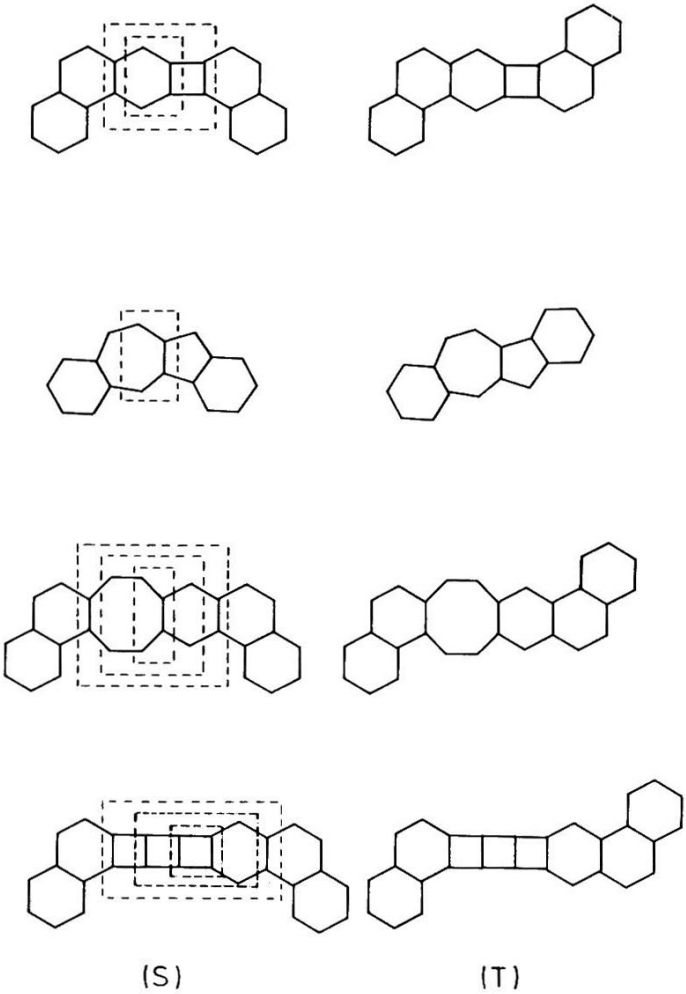


Figure 1: Some pairs of topomers S and T according to model 3, which satisfy eqs. (1) and (2). The possible C-moieties are indicated by rectangles; they are generated by C-formation using the subunits given in Table 2.

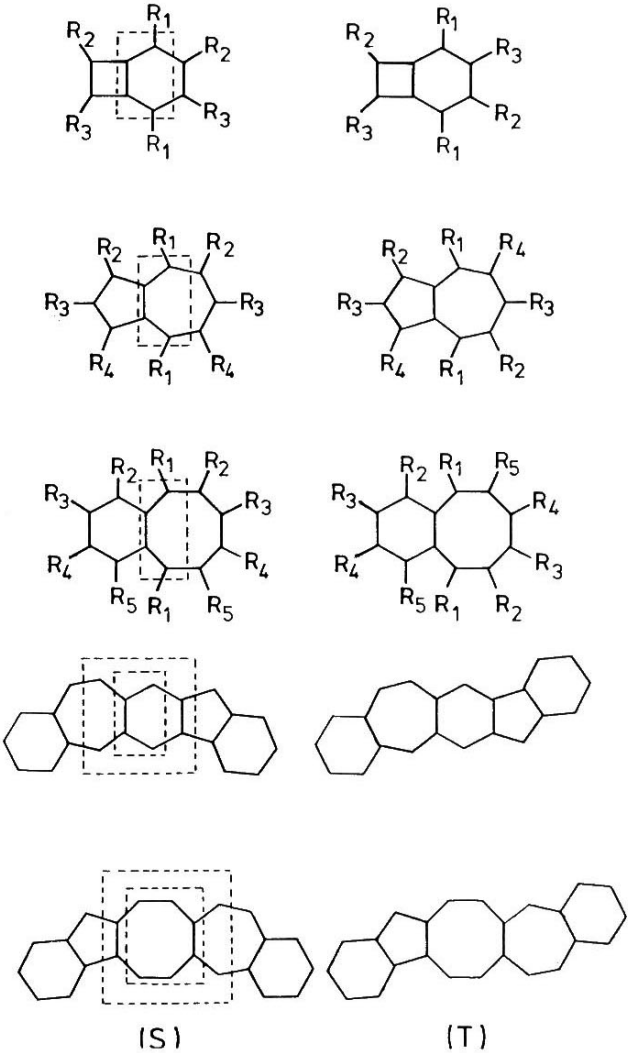
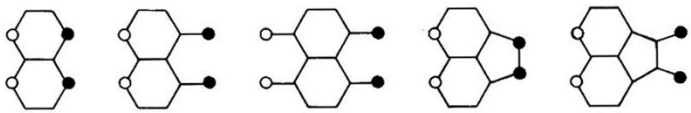


Figure 1 (cont.)

5. Discussion

When TEMO model 1 or 2 [2,7,10] is used in order to construct pairs of topomers satisfying eqs. (1) and (2) then their molecular graphs exhibit at least $S_2[E_n]$ symmetry; this is a consequence of the necessary demand for isomorphic subunits, A≈B, and a symmetric central moiety in case of model 2 [10]. In the event that the S and T topomers correspond to planar molecules then within these two models the S(T) topomer exhibits at least $C_{2v}(C_{2h})$ symmetry. In contrast the automorphism groups of all graphs shown in Figure 1 consist only of the identical mapping and have, therefore, order 1. Thus, the procedure described above offers access to topomers which possess lowest symmetry but, nevertheless, satisfy eqs. (1) and (2).

In an earlier paper [11] of this series it was observed that within some series of C-moieties the polynomial $C^{af} - C^{ae}$ does not alter. From the series given there we cite here the following one for which $C^{af} - C^{ae} = 3(x^2-1)$:



K_1, K_2, K_3, K_4, K_5.

It was said there: "In each member of a given series a certain 'kernel structure' is present which seems to determine the analytical form of $(C^{af} - C^{ae})$." Now, this observation is explained by the C-formation formalism: The graphs K_2 to K_5 may be generated from K_1, J_1, and J_2 by C-formation as follows

$$K_2 = K_1 \circledast J_1 \quad , \qquad K_3 = J_1 \circledast K_1 \circledast J_1 \quad ,$$

$$K_4 = K_1 \circledast J_2 \quad , \qquad K_5 = K_1 \circledast J_2 \circledast J_1 \quad .$$

As a consequence of that and of eq. (16) one obtains indeed

$$K_j^{af} - K_j^{ae} = K_1^{af} - K_1^{ae} = 3(x^2-1)$$

for j = 2,3,4,5. The "kernel structure" in this series is that of K_1. As seen from this example the generation of such a series from a given kernel structure can be performed by C-formation using an arbitrary number of subunits J_1 and/or J_2 but only those.

It should be mentioned that K_1 cannot be derived from G_0 and also cannot be generated from the F_j given in Table 2 by C-formation. K_1 belongs to a family of graphs treated in the subsequent note [16].

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