Generalized Wheland polynomial for large graphs

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We report the generalized Wheland polynomial for acyclic graphs depicting polyenes having $n = 10$ carbon atoms. We consider the problem of deriving generalized Wheland polynomials for larger chains by recursion. The recursion $\mathrm{Wh}(n+1;x) = \mathrm{Wh}(n;x) + (1-x)\mathrm{Wh}(n-1;x)$ allows one to find the next larger generalized Wheland polynomial for a chain having an even number of vertices by knowing generalized Wheland polynomials of chains having fewer vertices. The recursion, however, does not allow one to predict the generalized Wheland polynomial for a chain having an odd number of vertices from smaller chains! Here we report a procedure which allows one to derive the generalized Wheland polynomial for a chain having an odd number of vertices. This is achieved by combining the coefficients for rings having the same number of vertices. The generalized Wheland polynomials for odd rings are simply related to the generalized Wheland polynomials for smaller chains and can be derived from the information on smaller chains. This makes it possible to extend the recursion for generalized Wheland polynomials for arbitrarily large n.

1. Introduction

Conjugated systems, such as naphthalene illustrated in fig. 1, give rise to numerous valence structures. Besides the Kekule valence structures which depict coupling of pi-electrons at *adjacent* sites one can construct valence structures in which pi-electrons of nonadjacent carbon centers are coupled. The so-derived valence structures correspond to so-called "excited" valence structure or valence structures having "long bonds" (see fig. 1). The task of enumeration of structures of different degrees of "excitation", that is, having different numbers of "long bonds", is combinatorially difficult. In 1935 Wheland [1] introduced a powerful technique for enumeration of Kekule valence structures of "different degrees of excitation". It expresses the result in a form of a counting polynomial, that is, a polynomial whose coefficient for x^n represents the number of valence structures with n "long" bonds. If we recall that it was two years before Polya [2] published his famous counting theorem, the pioneering work of Wheland appeared as one of the first profound results in the emerging mathematical discipline of graph theory [3]. The counting polynomial of Wheland satisfies the recursive relation [1]

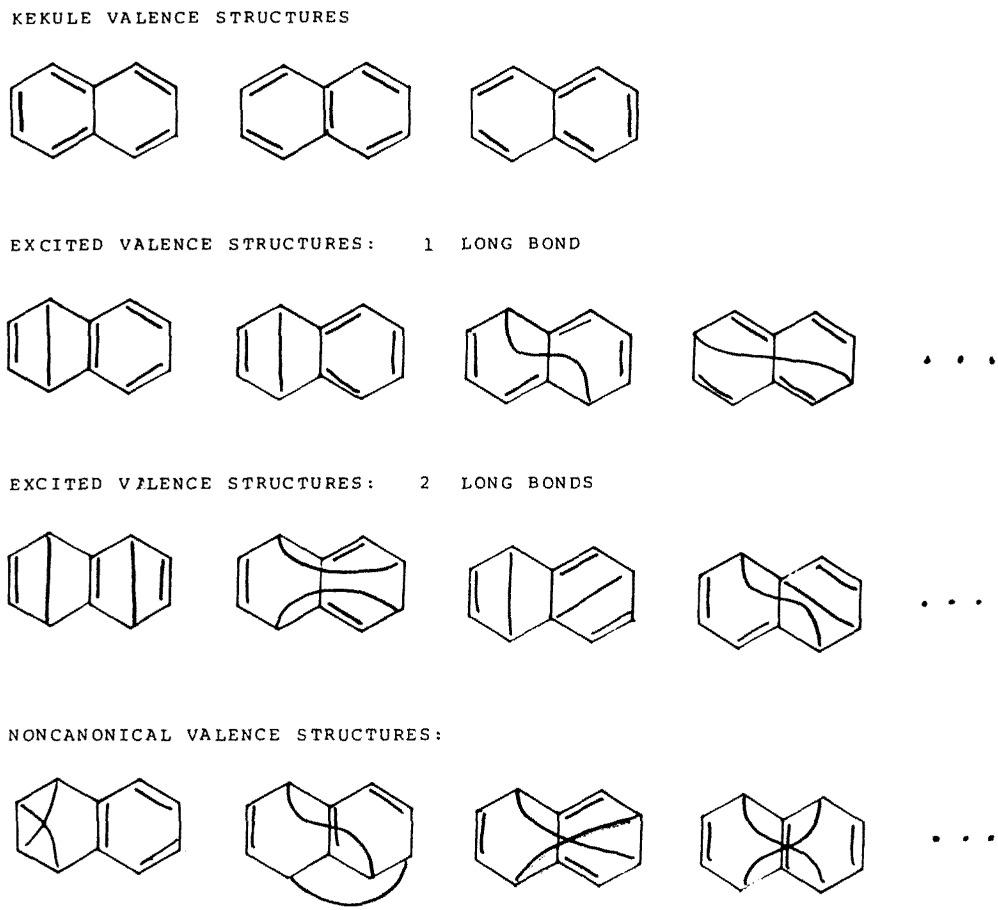

Fig. 1. Canonical valence structures of naphthalene of different degrees of excitation and selected noncanonical valence structures.

$$\mathrm{Wh}(G;x) = \mathrm{Wh}(G\text{–}E;x) + (1\text{-}x)\mathrm{Wh}(G\text{–}EE;x)\,,$$

where $G, G-E$, and $G-EE$ represent, respectively, a given graph, the graph with a single edge deleted, and the graph with all the adjacent edges to the edge E deleted. The enumeration that Wheland considered was carried out only over the *canonical* valence bond structures. In honoring George Wheland, we refer to this polynomial as the Wheland polynomial, Wh(x) [4,5]. While the Wheland polynomial appears to be an interesting structural function, it ought to be emphasized that it is not a structural *invariant*. The coefficients of the various powers of x in the polynomial depend on the selection of valence structures as the canonical, which depends on the selection of the labels for the vertices. Explicit forms of Wheland polynomials for chains are given in the book Chemical Graph Theory [6], while illustrations of polynomials can be found in refs. [7–10].

Is there a similar, mathematically related, counting polynomial which would represent a structural invariant, i.e. independent of the assumed labeling of vertices? In search for such an invariant, Randić and collaborators [4,5] considered *all* valence structures in their count, rather than restricting the count to the canonical "excited" structures. The new polynomial $\mathrm{GW}(G;x)$ is called the generalized Wheland polynomial, but the symbol GW could equally stand for George Wheland! In previous work GW polynomials were reported for chains and cycles up to $n = 18$, the results obtained by brute force of a computer. The program was outlined in refs. [4]. In a later publication [5] $\mathrm{GW}(G;x)$ were reported for many smaller graphs having less than $n = 8$ vertices. A relationship was found between the coefficients of GW and the nonadjacent numbers $p(G,k)$, which Hosoya [7] introduced in his study of the topological index for chemical structures. The $p(G,k)$ numbers satisfy a recursive relation [8], which thus allows one to derive the GW polynomials for longer chains recursively.

In this paper we report GW polynomials for trees having $n = 9$ and $n = 10$ vertices, including results for larger disconnected trees. We see however that the recursion of $\mathrm{GW}(G;x)$ for linear chains L_n, having n vertices,

$$\mathrm{Wh}(L_{n+1};x) = \mathrm{Wh}(L_n;x) + (1-x)\mathrm{Wh}(L_{n-1};x)\,,$$

holds only if $n+1$ is even! By using the above recursion, and by knowing GW polynomials for smaller chains, one can derive GW polynomials for the next largest even chain. But one cannot continue to find GW of the next odd chain since the recursion is not valid for odd chains. This appears somewhat peculiar and unsatisfactory. We could, as already mentioned, derive GW of a higher odd chain using properties of $p(G,k)$ and continue the next recursive step. Is it possible to resolve the peculiarity of GW polynomials for odd chains? We will outline an approach to recursion for GW of chains that does not involve $p(G,k)$ numbers. Instead it related the coefficients of GW polynomials for odd chains to those for odd rings. The GW for odd rings, however, can be derived from GW polynomials of smaller chains. The significance of this is that now one can derive GW for an arbitrary

Table 1
The generalized Wheland polynomials for acyclic structures having $n = 10$ vertices and perfect matching (that is, having a Kekule valence structure). The graphs are given in fig. 2.

1	$1 + 10x + 55x^2 + 185x^3 + 365x^4 + 329x^5$
2	$1 + 9x + 50x^2 + 191x^3 + 372x^4 + 322x^5$
3	$1 + 8x + 54x^2 + 185x^3 + 376x^4 + 321x^5$
4	$1 + 8x + 48x^2 + 188x^3 + 388x^4 + 312x^5$
5	$1 + 7x + 55x^2 + 188x^3 + 371x^4 + 323x^5$
6	$1 + 6x + 59x^2 + 182x^3 + 375x^4 + 322x^5$
7	$1 + 6x + 53x^2 + 185x^3 + 387x^4 + 313x^5$
8	$1 + 6x + 50x^2 + 194x^3 + 378x^4 + 316x^5$
9	$1 + 5x + 54x^2 + 188x^3 + 382x^4 + 315x^5$
10	$1 + 5x + 51x^2 + 197x^3 + 373x^4 + 318x^5$
11	$1 + 4x + 49x^2 + 194x^3 + 389x^4 + 308x^5$

graph and later use the relationship between GW and $p(G,k)$ to determine the latter. The nonadjacent numbers $p(G,k)$ in general are not easy to derive, except in special cases, such as linear chains.

2. Generalized polynomials for graphs with $N = 10$ vertices

In table 1 we have listed the generalized Wheland polynomials for the 11 graphs with ten vertices which correspond to all possible polyenes, i.e., trees having a (single) Kekule structure shown in fig. 2. The coefficient of the kth powers of the polynomials shows the number of valence structures with k "long" bonds (that is, k

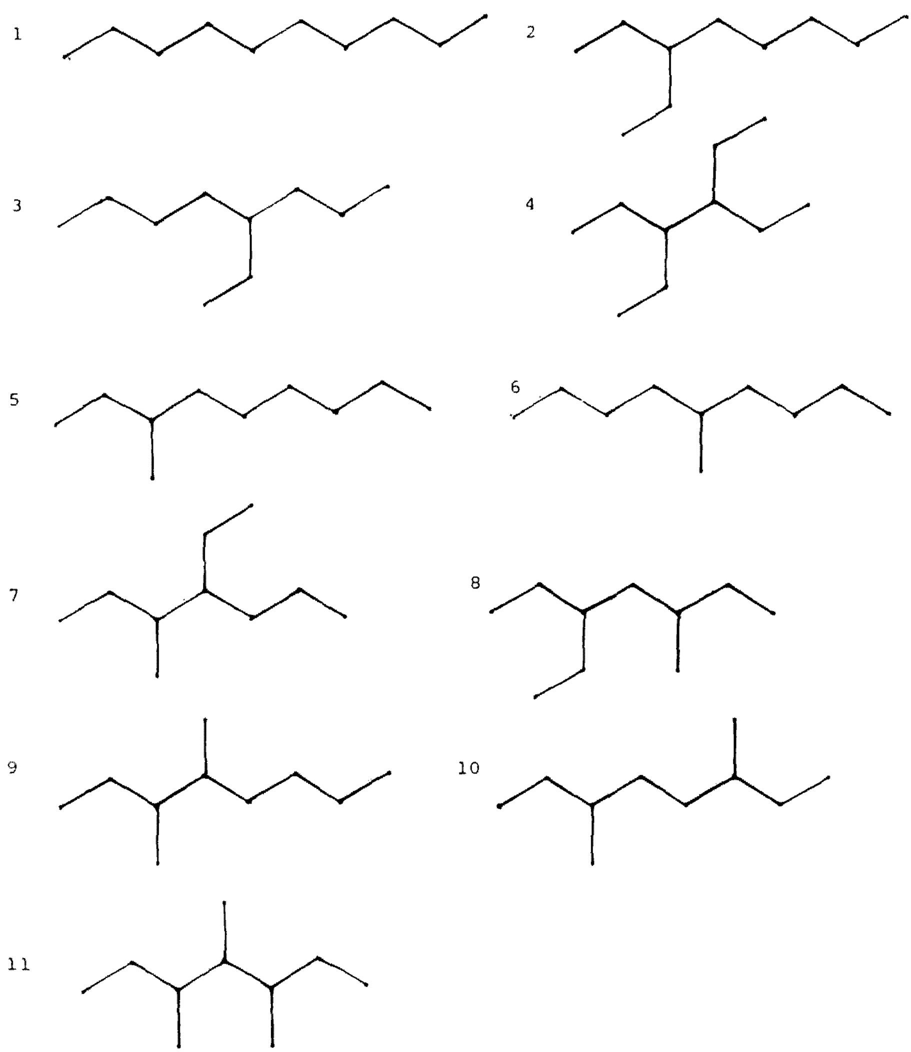

Fig. 2. Skeletons of polyenes having $n = 10$ carbon atoms and a Kekule structure.

is the "degree of excitation" of Wheland). The last coefficient (of the highest power) qualitatively shows the "degree of branching" of the molecular skeleton, the more "branched" the skeleton the smaller the coefficient.

In table 2 we have listed the generalized Wheland polynomials for acyclic systems having $n = 10$ vertices but with no Kekule structure. Hence there is no constant term in the GW polynomial in these cases. The structures 12–38 correspond to biradicals with two unpaired pi-electrons and to polyradicals (two structures) with four unpaired electrons. One can detect some regularity between the leading coefficient (the highest power of x) and the degree of branching. The structures 8 and 9 (fig. 3) represent a pair of isospectral graphs (that Schwenk has described [11]), and therefore we expect their generalized Wheland polynomials to be the same.

3. Disconnected graphs

The generalized Wheland polynomial for disconnected graphs cannot simply be derived from the knowledge of the polynomias for its parts as was the case for Whe-

Table 2
The generalized Wheland polynomials for acyclic structures having $n = 10$ vertices and no Kekule valence structure. The graphs are given in fig. 3.

1	$9x + 54x^2 + 189x^3 + 369x^4 + 324x^5$
2	$11x + 49x^2 + 192x^3 + 370x^4 + 323x^5$
3	$12x + 48x^2 + 189x^3 + 375x^4 + 321x^5$
4	$7x + 50x^2 + 198x^3 + 371x^4 + 319x^5$
5	$4x + 59x^2 + 189x^3 + 374x^4 + 319x^5$
6	$9x + 45x^2 + 201x^3 + 372x^4 + 318x^5$
7	$6x + 54x^2 + 192x^3 + 375x^4 + 318x^5$
8	$8x + 49x^2 + 195x^3 + 376x^4 + 317x^5$
9	$8x + 49x^2 + 195x^3 + 376x^4 + 317x^5$
10	$5x + 58x^2 + 186x^3 + 379x^4 + 317x^5$
11	$7x + 53x^2 + 189x^3 + 380x^4 + 316x^5$
12	$9x + 548x^2 + 192x^3 + 381x^4 + 315x^5$
13	$11x + 43x^2 + 195x^3 + 382x^4 + 314x^5$
14	$4x + 50x^2 + 201x^3 + 377x^4 + 313x^5$
15	$6x + 45x^2 + 204x^3 + 378x^4 + 312x^5$
16	$63x^2 + 186x^3 + 384x^4 + 312x^5$
17	$5x + 49x^2 + 198x^3 + 382x^4 + 311x^5$
18	$4x + 53x^2 + 192x^3 + 386x^4 + 310x^5$
19	$6x + 48x^2 + 195x^3 + 387x^4 + 309x^5$
20	$8x + 43x^2 + 198x^3 + 388x^4 + 308x^5$
21	$7x + 47x^2 + 192x^3 + 392x^4 + 307x^5$
22	$4x + 56x^2 + 183x^3 + 395x^4 + 307x^5$
23	$4x + 44x^2 + 204x^3 + 389x^4 + 304x^5$
24	$60x^2 + 180x^3 + 405x^4 + 300x^5$

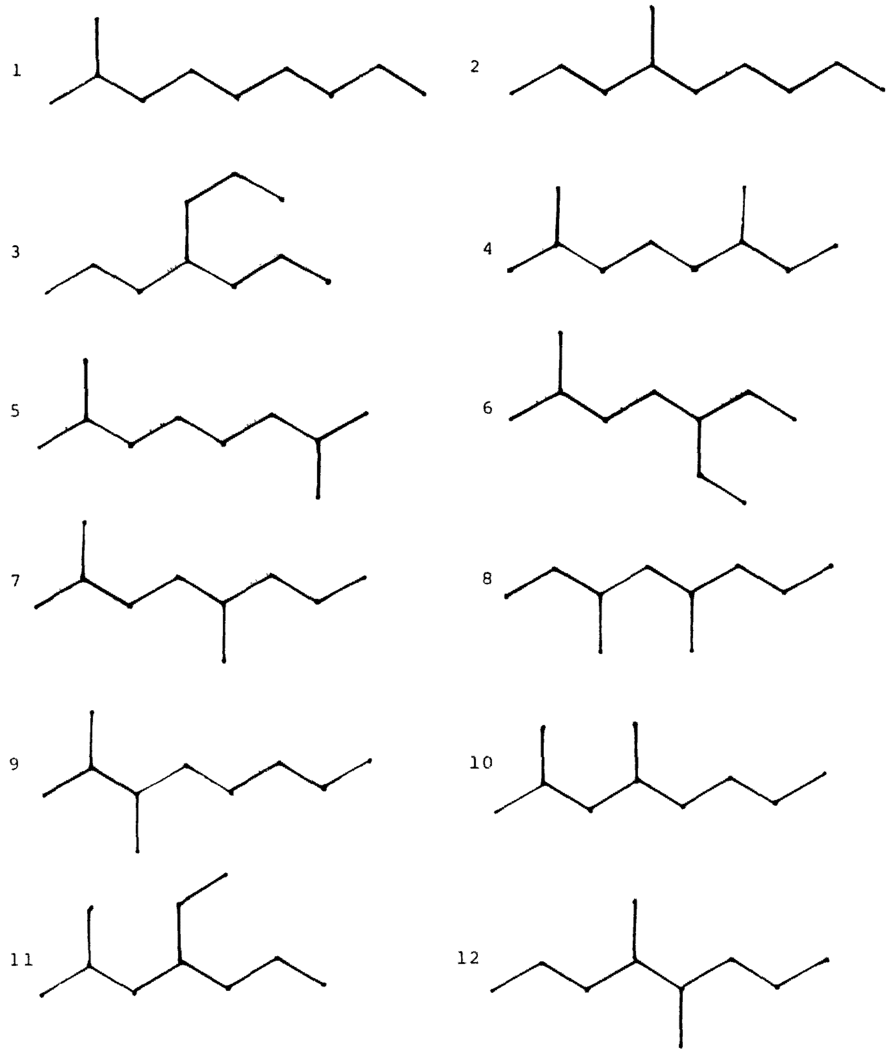

Fig. 3. (Continues.)

land polynomials. In ref. [4] this was illustrated for the naphthalene graph showing cases in which the recursion for GW(x) was valid or not valid. The recursion holds for GW(x) only if the recursion produces graphs with a single component, that is, graphs *G-E* and *G-EE*, are connected, as has been observed in refs. [4]. This clearly suggests that *disconnected* components cannot be considered independently. That is, the GW of a graph having two components is not simply given as the product of GW's of the two component, as has been the case with Wh(x).

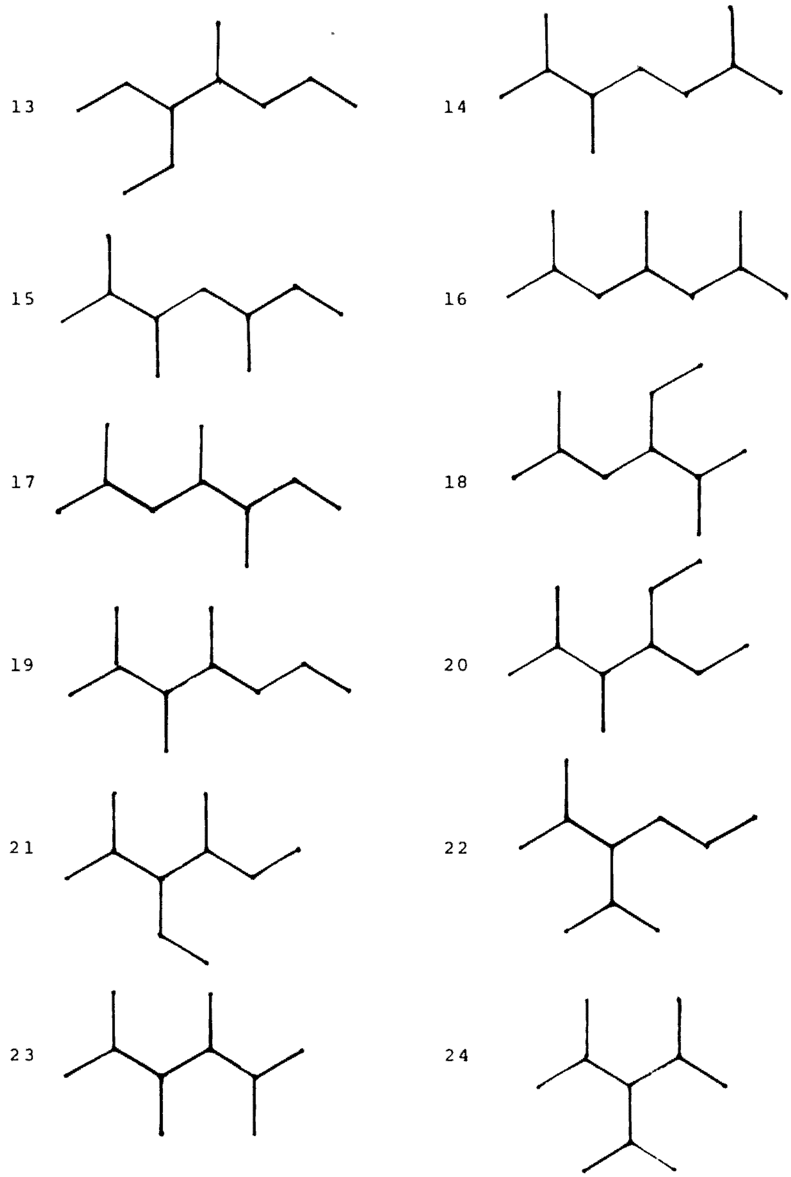

Fig. 3. Acyclic graphs having $n = 10$ vertices and no Kekule structure.

In fig. 4 we illustrate the correspondence between valence structures of a chain of six vertices (hexatriene), the valence structures of a disconnected chain on six vertices (bond 2-3 is missing), and the valence structure of a chain with five vertices but having six pi-electrons (a radical). The first column gives all the 15 valence structures of different degrees of excitation possible for hexatriene in the central column we show the corresponding structures for the case in which the bond 2-3

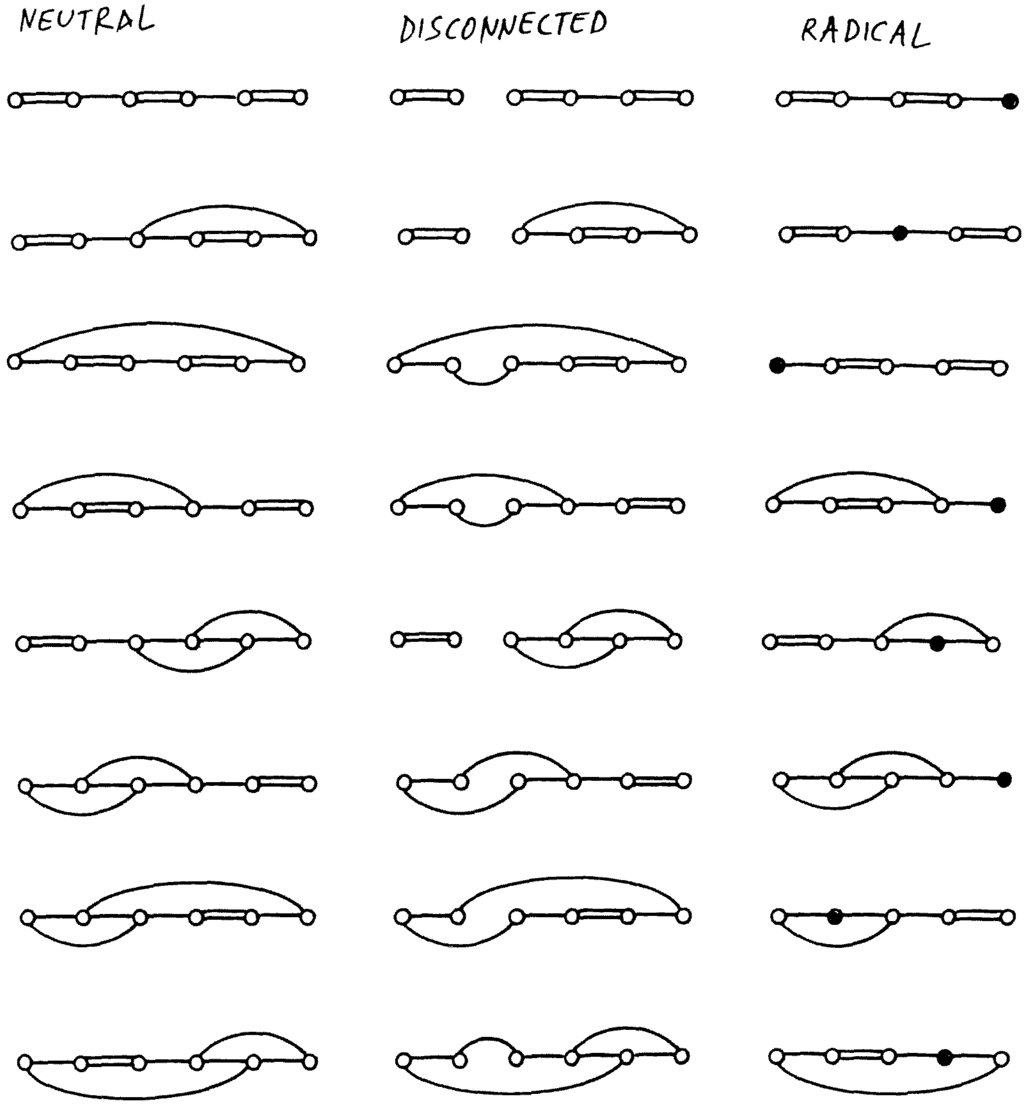

Fig. 4. (continues).

was erased, i.e., for the disconnected chain composed of ethylene and butadiene. The last column illustrates a reduction of a coupling of a pair of pi-electrons in a six-vertex chain to a single uncoupled electron in a five-vertex chain.

The count of valence structures in the disconnected graph is simply related to the count of the valence structures of the hexatriene: All structures in which the erased bond 2-3 was a single CC bond make the same contribution to the generalized Wheland polynomial as before. All structures in which the erased bond 2-3 was a double CC bond formally have increased the degree of excitation. A net effect of

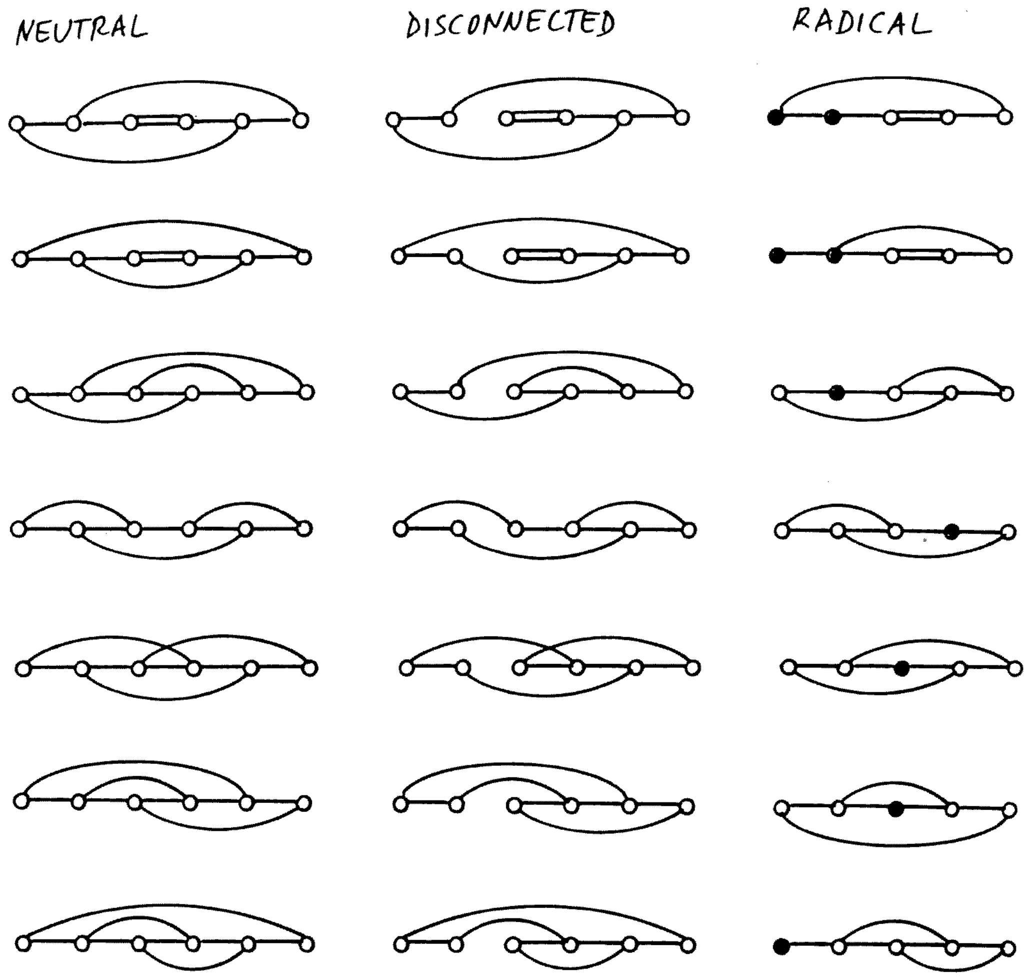

Fig. 4. All 15 possible valence structures of hexatriene, the corresponding valence structures for a graph obtained by erasure of bond 2-3, and the corresponding valence structures for a graph obtained by erasure of a terminal vertex, converting the corresponding valence structures involving an uncoupled pi-electron to radical valence structures.

this is that the number of valence structures of lower excitation decreases somewhat while the number of valence structures of the higher excitation increases. Thus from fig. 4 we see that for hexatriene two of the single excited structures are transformed into doubly excited structures, making a change of $-2x + 2x^2$ to the polynomial, while one of the doubly excited valence structure becomes a triply excited structure causing a change in the polynomial $-x^2 + x^3$, making the overall change of $-2x + x^2 + x^3$. Thus instead of

$$1 + 3x + 6x^2 + 5x^3$$

Table 3
The generalized Wheland polynomials for linear chains having disconnected components.

n	Deleted	Generalized Wheland polynomial coefficients							
		Const.	x	x^2	x^3	x^4	x^5	x^6	x^7
4	1–2	0	2	1					
	2–3	1	0	2					
6	1–2	0	3	6	6				
	2–3	1	1	7	6				
	3–4	0	4	4	7				
8	1–2	0	4	18	42	41			
	2–3	1	3	18	41	42			
	3–4	0	6	15	42	43			
	4–5	1	2	21	38	43			
10	1–2	0	5	40	165	370	365		
	2–3	1	6	41	161	366	370		
	3–4	0	8	40	162	364	371		
	4–5	1	4	46	158	365	371		
	5–6	0	9	36	168	360	372		
12	1–2	0	6	75	480	1830	4020	3984	
	2–3	1	10	85	485	1850	3989	4020	
	3–4	0	10	85	490	1805	3980	4025	
	4–5	1	7	88	488	1808	3977	4026	
	5–6	0	12	78	498	1803	3978	4026	
14	1–2	0	7	126	1155	6580	23940	51828	51499
	2–3	1	15	162	1240	6630	23724	51535	51828
	3–4	0	12	156	1245	6660	23730	51468	51864
	4–5	1	11	156	1240	6665	23739	51454	51869
	5–6	0	15	150	1245	6660	23745	51450	51870
	6–7	1	9	165	1225	6675	23739	51451	51870
	7–8	0	16	144	1260	6640	23760	51444	51871

for GW$(G;x)$ of hexatriene we obtain

$$1 + x + 7x^2 + 6x^3$$

for GW$(G;x)$ of the disconnected chain having $n = 6$ vertices and bond 2-3 missing.

The knowledge of GW for a chain having disconnected parts is of considerable interest when applied to the recursion relation for GW. Acyclic structures and acyclic fragments of cyclic structures always lead to disconnected fragments unless terminal vertices are employed. In table 3 we have therefore listed GW$(G;x)$ for disconnected even linear chains having $n = 14$ or fewer vertices.

4. Linear chains having an odd number of vertices

Structures having an odd number of vertices necessarily have $K = 0$, i.e., have no (unexcited) Kekule structure. Their $GW(G; x)$ will have no constant term. The coefficient of x in $GW(G; x)$ now counts the number of Kekule valence structures for the radical. This is illustrated in fig. 5 for a few structures having $n = 9$ vertices. Table 4 lists the $GW(G; x)$ for 18 acyclic structures with $n = 9$ (illustrated in fig. 6). See that the sum of the coefficients in structures having an odd number of vertices, $2k - 1$, is the same as for structures having $2k$ vertices. While this suggests

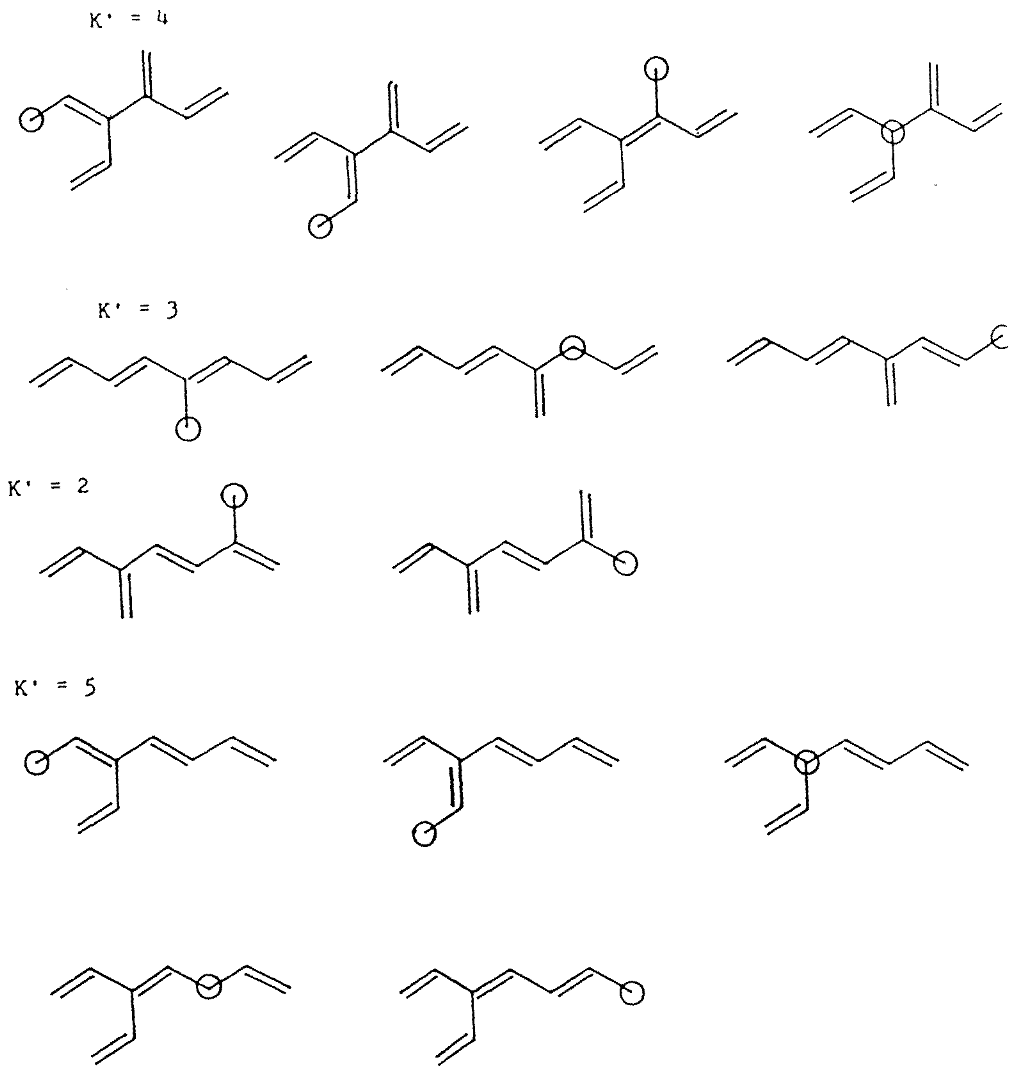

Fig. 5. Selected graphs having $n = 9$ vertices for which erasure of a single vertex gives rise to different values for K' (the coefficient of the linear term in $GW(G; x)$).

Table 4
The generalized Wheland polynomials for acyclic structures having $n = 9$ vertices. The graphs are given in fig. 6.

1	$5x + 40x^2 + 165x^3 + 370x^4 + 365x^5$
2	$2x + 40x^2 + 168x^3 + 376x^4 + 359x^5$
3	$4x + 35x^2 + 171x^3 + 377x^4 + 358x^5$
4	$3x + 39x^2 + 165x^3 + 381x^4 + 357x^5$
5	$5x + 34x^2 + 168x^3 + 382x^4 + 356x^5$
6	$4x + 38x^2 + 162x^3 + 386x^4 + 355x^5$
7	$2x + 31x^2 + 180x^3 + 379x^4 + 353x^5$
8	$3x + 30x^2 + 172x^3 + 384x^4 + 351x^5$
9	$39x^2 + 168x^3 + 387x^4 + 351x^5$
10	$2x + 34x^2 + 171x^3 + 388x^4 + 350x^5$
11	$2x + 34x^2 + 171x^3 + 388x^4 + 350x^5$
12	$2x + 37x^2 + 162x^3 + 397x^4 + 347x^5$
13	$3x + 32x^2 + 165x^3 + 398x^4 + 346x^5$
14	$30x^2 + 180x^3 + 390x^4 + 345x^5$
15	$36x^2 + 162x^3 + 408x^4 + 399x^5$

that the two are related, it also suggests that one should not expect the recursion to yield the GW polynomials for the case $2k + 1$, which will have $2k + 1$ times more terms. The total number of valence structures, i.e., the sequence: 1, 3, 15, 105, 945, 10395, ... represents "odd" factorials $(2k\text{-}1)!!$ [5].

The observation that graphs on $2k$ and $2k - 1$ vertices have the same number of valence structures suggests that we try to derive the count of valence structures of different excitation for the case of graphs having an odd number $2k - 1$ of vertices by considering the valence structures of graph having $2k$ vertices. This is illustrated in the last column of fig. 4 where a single terminal vertex of hexatriene is dropped. The dropped vertex results in a presence of an uncoupled pi-electron. In such trees the coefficient in $GW(G; x)$ of the linear term, again, as the constant term in graphs with an even number of vertices, counts the number of Kekule structures of the corresponding radical (as previously illustrated in fig. 5 by few examples for the case $n = 9$). This coefficient can be derived independently by a graphical procedure (outlined elsewhere [12]), which is particularly of interest in polycyclic systems which may have many such radical Kekule structures.

5. Recursion

In table 5 we have collected the coefficients of GW for even and odd linear chains separately. Knowing the limitations of the recursive formula, which does not allow one from knowing the coefficients for chains having $2k$ vertices to find the coefficients for a chain having $2k + 1$ vertices, the question is then that of trying to find recursion for either only even or only odd linear chains. The problem, how-

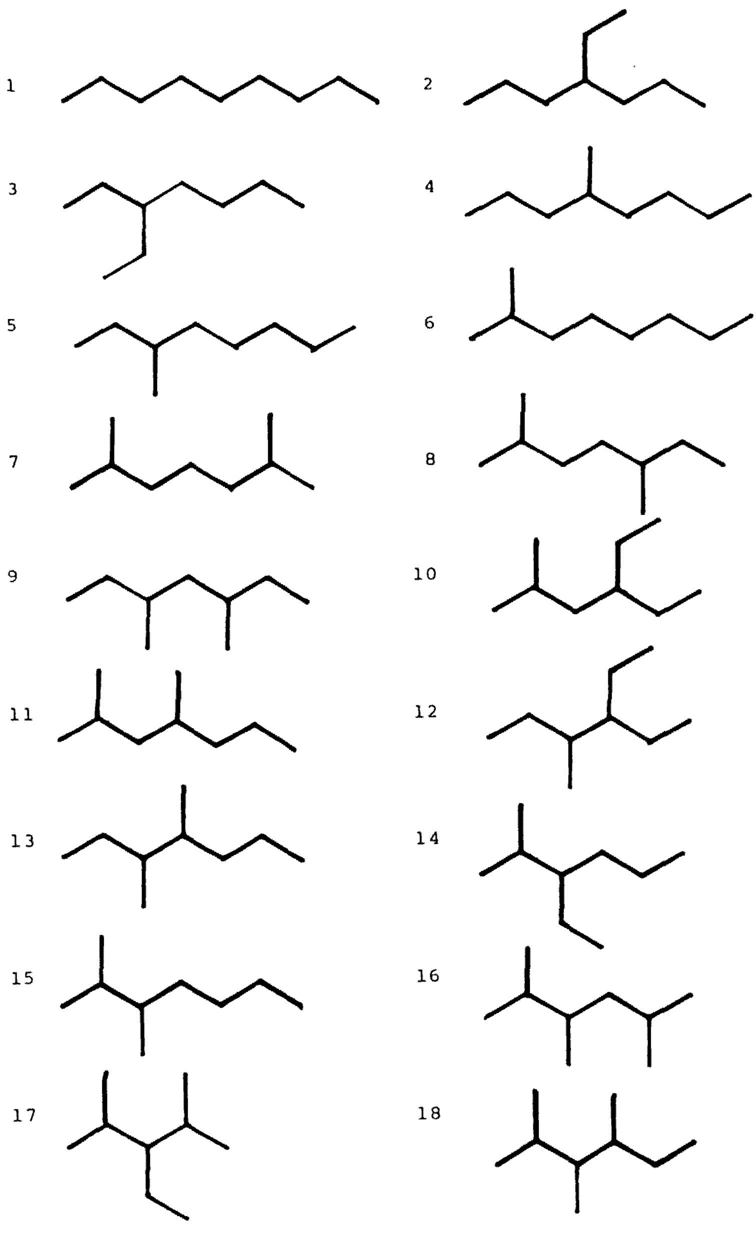

Fig. 6. Molecular diagrams for polyene radicals having $n = 9$ vertices.

ever, appears unsurmountable because the size of the coefficients dramatically increases when going from graphs having $2k$ vertices to graphs having $2k + 1$ vertices. The increment is given by the factor $(2k + 1)$ itself, as shown earlier. As is not uncommon in mathematics, the difficulty of some problems may increase when one restricts the scope of the problem. The solution to our problem becomes simple

Table 5
The generalized Wheland polynomials for chains having even and odd numbers of atoms, and rings having an odd number of atoms.

Even chains:	
$n = 2$	1
$n = 4$	$1 + x + x^2$
$n = 6$	$1 + 3x + 6x^2 + 5x^3$
$n = 8$	$1 + 6x + 21x^2 + 41x^3 + 36x^4$
$n = 10$	$1 + 10x + 55x^2 + 185x^3 + 365x^4 + 329x^5$
...	...
Odd chains:	
$n = 3$	$2x + x^2$
$n = 5$	$2x + 6x^2 + 6x^3$
$n = 7$	$4x + 18x^2 + 42x^3 + 41x^4$
$n = 9$	$5x + 40x^2 + 165x^3 + 370x^4 + 365x^5$
...	...
Odd rings:	
$n = 3$	$3x$
$n = 5$	$5x(1 + x + x^2)$
$n = 7$	$7x(1 + 3x + 6x^2 + 5x^3)$
$n = 9$	$9x(1 + 6x + 21x^2 + 41x^3 + 36x^4)$
...	...

when we extend the consideration to ring structures. Ring structures should have been expected to be "simpler" compared to chains in view of the "equivalence" of all vertices in the construction of Rumer diagrams [13] for these. The Rumer diagrams illustrate the pairing of pi-electrons for the canonical valence structures only, that is, they are subject to the "noncrossing" rule for the couplings. The equivalence of vertices, of course, breaks down in chains. While a regularity in the coefficients of even rings is not apparent, the coefficients of $\mathrm{GW}(G; x)$ for odd rings show a rather simple structure. When the common factor $2k + 1$ is factored out the reduced coefficients are those of linear chains of size $2k$. Thus from the information on a *smaller* chain we can derive $\mathrm{GW}(x)$ for a *larger* ring. However, from a ring we can always get $\mathrm{GW}(G; x)$ for the chain of the *same* size! Hence by combining the above two steps we can extend the recursion for $\mathrm{GW}(G; x)$ to chains of ever increasing size. In table 6 we illustrate for a chain of length $n = 9$, how one can derive GW knowing GW for a ring having nine vertices and shorter chains.

6. Concluding remarks

Generalizing the recursion for $\mathrm{GW}(G; x)$ is a useful novel result. Construction of $\mathrm{GW}(G; x)$ for larger graphs previously was limited by the computational complexity of the brute force calculations. With the outlined construction we extended the size of graphs for which GW can be constructed. Moreover one can use the con-

Table 6
Construction of the generalized Wheland polynomial for a chain of length $n = 9$ using the information on $GW(x)$ for a ring with nine atoms and smaller chains.

Ring(9) = Chain(9) + $(1 - x)$ Chain(7)

Hence

Chain(9) = Ring(9) − $(1 - x)$ Chain (7)
= $9x$ Chain(8) − $(1 - x)$ Chain(7)

Thus:

$$\begin{array}{r} 9x(1 + 6x + 21x^2 + 41x^3 + 36x^4) \\ +(x-1)(\quad 4x + 18x^2 + 42x^3 + 41x^4) \\ \hline \end{array}$$

Chain(9): $5x + 40x^2 + 165x^3 + 370x^4 + 365x^5$

structed $GW(G; x)$ to derive $p(G, k)$ numbers for larger graphs using the relationship between the two [5]. Direct use of computers to obtain GW for large graphs is practically limited already for graphs of size less than $n = 20$. For example, graphs having $n = 16$ vertices require over 3.5 hours of CPS on a VAX 11/780 computer to obtain generalized Wheland polynomials. Graphs having $n = 18$ vertices increase the computation time to over 90 hours! A hope that one will be able to compute $GW(G; x)$ for larger graphs by a computer therefore appears unpromising.

Admittedly, $GW(G; x)$ have also a rather limited direct application, but their relationship to $p(G, k)$ opens up novel use. The $p(G, k)$ are the coefficients of the acyclic or matching polynomial [14]. They are of interest in structure–property correlations in chemistry [15]. Their evaluation in a general case is rather tedious, particularly for large systems, unless there is some symmetry. For translational symmetry in linearly fused benzenes the technique of the transfer matrix [16] can be successively applied [17], while for an arbitrarily linearly fused benzene ring system one has to use several such matrices [18]. The present approach, which allows an extension of the use of the recursion, makes it possible to use the relationship between $GW(x)$ and $p(G, k)$ to derive the latter in a relatively straightforward way.

The presentation also illustrate the benefits, not unknown in mathematical studies, where a problem is simplified by considering a more general case. By considering ring and chain structures jointly, rather than separately, we were able to derive useful recursion. If one would have focused attention to the ring structures alone again one would not have been able to successfully derive the recursion and extend the results for smaller rings to construction of the generalized Wheland polynomials for large rings.

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