

## Note on Algebraic Structure Count

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An efficient graphical method for the calculation of algebraic structure count is presented which is an alternative to the method proposed by Gutman and is a generalization of the method of Randić.

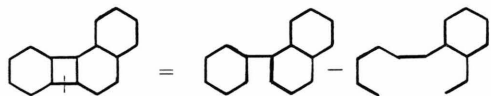
The number of Kekulé structures ( $K$ ) of an even alternant molecular graph ( $G$ ) can be easily calculated by means of the following recursion formula due to Randić:

$$K(G) = K(G-e) + K(G-(e)), \quad (1)$$

where  $G-e$  is the graph obtained upon deletion of edge  $e$ , and  $G-(e)$  is the graph obtained upon deletion of  $e$  along with its associated vertices [1]. Gutman stated that "... no analogous regularity has been previously observed for the algebraic structure count" [2]. For alternant molecular graphs possessing only  $4n+2$  rings ( $n$ =integer),  $K(G) = \text{ASC}(G)$ . We now show that the following recursion, which is a generalization of (1), is applicable to alternant molecular graphs possessing  $4n$  rings:

$$|\text{ASC}(G)| = |\text{ASC}(G-e) \pm \text{ASC}(G-(e))|, \quad (2)$$

where the negative sign is only chosen when  $e$  belongs solely to a  $4n$  ring. In the application of the recursion (2), one needs to remember that  $K=2$  and  $\text{ASC}=0$  for both antiaromatic cyclobutadiene and cyclooctatetraene (or other  $4n$  monocyclic rings). The reader should compare this simpler method with that of Gutman [2, 3]. Using the structure, benzo[*a*]biphenylene, given in his paper [2], one can quickly show by (2) that  $|\text{ACS}| = 3 \cdot 2 - 2 = 4$  by operating on either of the perimeter cyclobutadiene edges.



$$\text{ASC}(b[a]b) = 2 \cdot 3 - 2 = 4.$$

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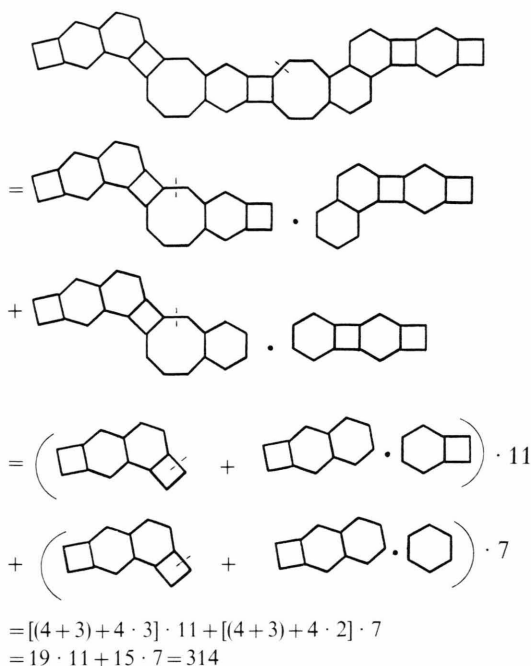


Fig. 1 a. Recursive application of  $K(G) = K(G-e) + K(G-(e))$ .

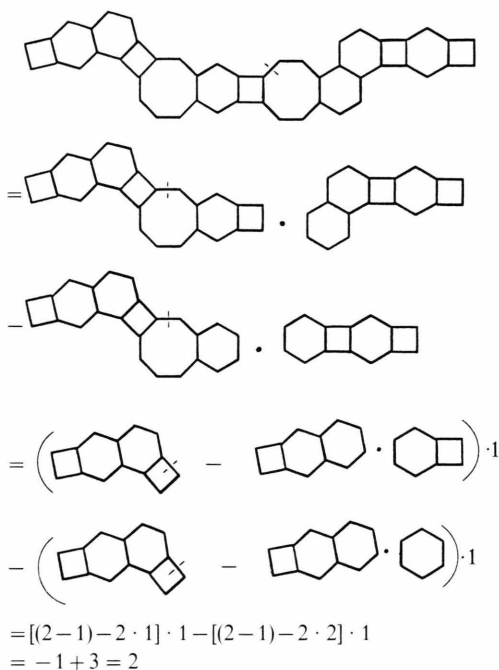


Fig. 1 b. Recursive application of  $\text{ASC}(G) = |\text{ASC}(G-e) \pm \text{ASC}(G-(e))|$ .

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As a further demonstrative example, consider a recent structure (Figure 1) presented by Klein and coworkers having  $K = 314$  and  $|\text{ASC}| = 2$ , which they determined by a matrix transfer method [4]. Note that the initial edges operated on are marked and that we automatically omit all the essential double bonds in the decomposition process. Successive application of (1) gives  $K = 314$ , and successive application of (2) gives  $|\text{ACS}| = 2$  as shown in Figure 1.

These recursive equations are also applicable to peri-condensed molecular graphs. Thus, (2) represents a generalization of the method of Randić and represents an important improvement since ASC is widely used in structure-resonance theory [5] and conjugated circuit determination of resonance energies [6]. While the matrix transfer method of Klein and coworkers [4] holds for only catacondensed-like systems, the present approach is more general and is particularly useful for alternant systems composed of a single  $4n$  ring.

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