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.

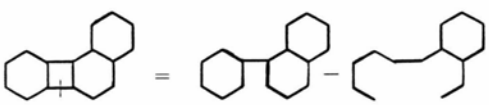
The number of Kekulé structures (K) of an even alternant molecular graph (G) can be easily calculated by means of the following recursion formula due to Randić:

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

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), $K(G) = \mathrm{ASC}(G)$. We now show that the following recursion, which is a generalization of (1), is applicable to alternant molecular graphs possessing $4n$ rings:

$$|\mathrm{ASC}(G)| = |\mathrm{ASC}(G-e) \pm \mathrm{ASC}(G-(e))|, \qquad (2)$$

where the negative sign is only chosen when e belongs soley to a $4n$ ring. In the application of the recursion (2), one needs to remember that $K=2$ and $\mathrm{ASC}=0$ 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 $|\mathrm{ACS}| = 3\cdot 2 - 2 = 4$ by operating on either of the perimeter cyclobutadiene edges.



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

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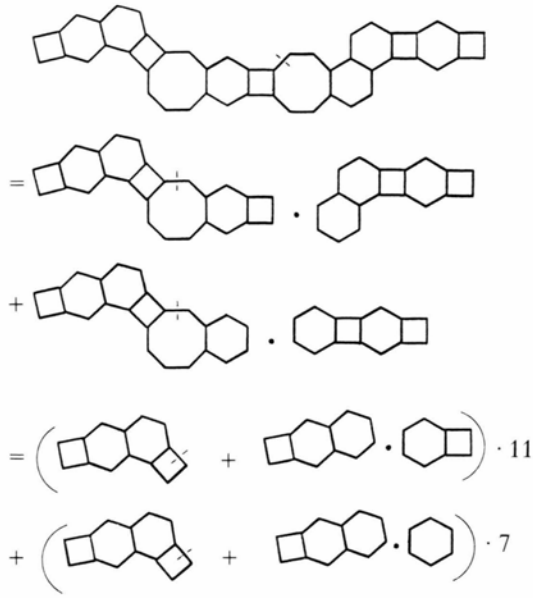
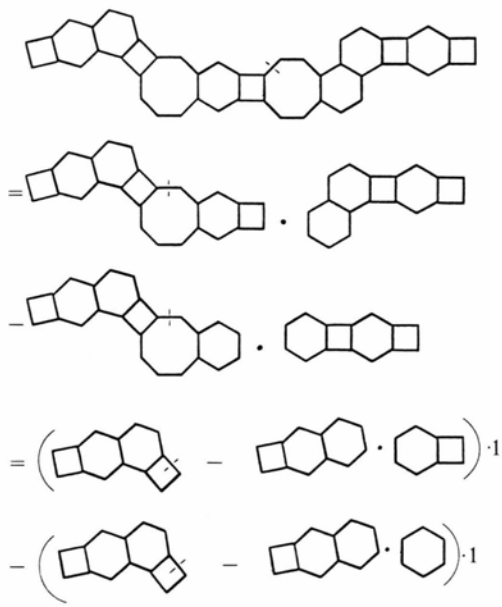


$= [(4+3)+4\cdot 3]\cdot 11 + [(4+3)+4\cdot 2]\cdot 7$
$= 19\cdot 11 + 15\cdot 7 = 314$

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



$= [(2-1)-2\cdot 1]\cdot 1 - [(2-1)-2\cdot 2]\cdot 1$
$= -1+3 = 2$

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

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As a further demonstrative example, consider a recent structure (Figure 1) presented by Klein and coworkers having $K = 314$ and $|ASC| = 2$, 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 $|ACS| = 2$ 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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