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 Randic.

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:

\[
K(G) = K(G - e) + K(G - (e)), \tag{1}
\]

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

\[
|\text{ASC}(G)| = |\text{ASC}(G - e) \pm \text{ASC}(G - (e))|, \tag{2}
\]

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 \( |\text{ASC}| = 3 \cdot 2 - 2 = 4 \) by operating on either of the perimeter cyclobutadiene edges.

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

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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.