The Number of Kekulé Structures of Hexagon-shaped Benzenoids and Members of Other Related Classes

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Some results from the enumeration of Kekulé structures are reviewed; they pertain to parallelogram-shaped, bent strips, chevrons and symmetrical hexagon-shaped benzenoids. The existing formulas are extended to the class of asymmetrical hexagons. Applications of the new formula reproduces a number of known results for three-tier and four-tier strips. In the latter case also some new formulas are achieved.

(Keywords: Kekulé structures; Benzenoids)

Die Anzahl der Kekulé-Strukturen von Benzenoiden mit sechseckigem Umriß und Mitgliedern anderer verwandter Klassen

Es wird ein Überblick über die Berechnung der Anzahl möglicher Kekulé-Strukturen von benzenoiden Verbindungen unterschiedlicher Formenklassen gegeben. Dabei werden die existierenden Formeln für die Klasse asymmetrischer Sechseckformen ausgeweitet und die neue Formel auch an bekannten Ergebnissen erprobt.

Introduction

The enumeration of Kekulé structures in conjugated hydrocarbons has attained an increasing interest in modern times. The present work deals with peri-condensed benzenoid systems only; they are represented by reticles of regular hexagons. The emphasis is laid on combinatorial formulas in closed form. The number of Kekulé structures of a benzenoid B is designated $K\{B\}$.

The main subject of this paper is a study of a class of benzenoids referred to as hexagonal. We prefer this designation rather than the alternative "circular", especially because we now are going to renounce much of the symmetry in these systems.
Results and Discussion

Previous Results

The combinatorial formula of $K$ for the $m \times n$ parallelogram-shaped benzenoids, say $L(m, n) = L(n, m)$, is a classical result\(^7\), which has been quoted frequently\(^4-6,8\):

$$K\{L(m, n)\} = \binom{m+n}{n} \quad (1)$$

This class of benzenoids contains two parameters $(m,n)$, which are the numbers of hexagons in a row or column. In general the parameters are positive integers, which however, usually may degenerate to zero. Classes of three-parameter benzenoids have also been studied:

1. Bent strip. This (V-shaped) benzenoid may be interpreted as a sub-benzenoid of the $m \times n$ parallelogram; cf. Fig. 1. It is determined by three parameters $(k, m, n)$. A general formula for the number of Kekulé structures has recently been derived by Cyvin and Gutman\(^9\);

$$K\{V(k, m, n)\} = \sum_{i=0}^{k} \binom{m}{i} \binom{n}{i} \quad (2)$$

These authors\(^9\) have also solved the problem for the bent strip of unequal thickness of the two branches, a four-parameter problem.

2. Chevron-shaped benzenoids. The classical paper of Gordon and Davison\(^7\) contains a general formula for the $K$ number of a three-parameter chevron-shaped benzenoid; cf. Fig. 2. The formula has since