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Algebraic Kekul Structures of Benzenoid Hydrocarbons ...

An algebraic Kekul structure of a benzenoid hydrocarbon is obtained from an ordinary Kekul structure by inscribing into each hexagon the number of π -electrons which (according to this Kekul structure) belong to this hexagon. Kekul Structures in Benzenoid Hydrocarbons | Sven J ...

This text is an attempt to outline the basic facts concerning Kekul structures in benzenoid hydrocarbons; their history, applications and especially enumeration.

[Lecture Notes in Chemistry] Kekul Structures In Benzenoid ...

Several typical examples are found among the all-benzenoid classes, both catacondensed (Section 6.5) and pericondensed (Chapter 16). We are inclined to give Randić (1980) the credit for a first systematic treatment of the number of Kekule structures (X) for benzenoid systems with repeated units.

Binary Coding of Kekul Structures of Catacondensed

An algorithm is described by means of which the Kekul structures of a catacondensed benzenoid molecule (with h hexagons) are transformed into binary codes (of length h). KEKULI- STRUCTURES AND THEIR SYMMETRY PROPERTIES - core.ac.uk

Kekul6 structures (K), especially in the theoretical chemistry of benzenoid hydrocarbons. Some Some of the most important practical applications of the Kekul6 structures, and their number K in

Algebraic Kekul Structures of Benzenoid Hydrocarbons ...

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Kekul structures and their symmetry properties - [PDF ...

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(PDF) Benzenoid isomers with greatest and smallest Kekul ...

The applicability of the Hall rule (linear relation between the total π -electron energy and the number of Kekul structures) was investigated in the case of fluoranthene-type benzenoid hydrocarbons.

Binary coding of Kekulé structures of catacondensed

...

$R(G)$ of the benzenoid hydrocarbon B are the Kekulé structures of B ; two vertices of $R(G)$ are adjacent if the corresponding Kekulé structures interact, that is if they differ in the position of just three double bonds.

Determining the Number of Resonance Structures in ...

The number of resonance structures (SC) for previously published concealed non-Kekulé benzenoid hydrocarbons is determined. Using a simple computer program, analytical expressions for determining SC for various classes of non-Kekulé (free-radical) benzenoid hydrocarbons are derived, and some properties of concealed non-Kekulé benzenoid