Finding a Bijection Between the Kekulé Structures of Benzenoids and Weakly Increasing Matrices

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Benzenoids are organic compounds composed of hexagonal six-carbon benzene rings with no adjacent double bonds. A Kekulé structure models a benzenoid as a collection of selected edges (representing double bonds) such that every vertex (representing a carbon atom) is paired with exactly one other vertex. Weakly increasing matrices are matrices whose entries are non-decreasing along every row and column. This research establishes a bijection between the set of Kekulé structures for certain hexagonal benzenoids and the set of two-row weakly increasing matrices with bounded integer entries. This bijection admits a geometrically intuitive interpretation and yields a compact encoding of these benzenoids. More broadly, this matrix-based perspective may open new directions in computational chemistry including faster simulations, improved representations for machine learning, and new approaches to molecular design.

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