The Structural Information Content of Chemical Networks

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We present an information-theoretic method to measure the structural information content of networks and apply it to chemical graphs. As a result, we find that our entropy measure is more general than classical information indices known in mathematical and computational chemistry. Further, we demonstrate that our measure reflects the essence of molecular branching meaningfully by determining the structural information content of some chemical graphs numerically.

Key words: Structural Information Content; Graph Entropy; Information Theory; Chemical Graph Theory.