

The structural information content of chemical networks

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Abstract

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.

Keywords

Chemical graph theory; Graph entropy; Information theory; Structural information content

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