

ENTROPY DUE TO FRAGMENTATION OF DENDRIMERS

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Abstract. Subgraphs can results through application of criteria based on matrix which characterize the entire graph. The most important categories of criteria are the ones able to produce connected subgraphs (fragments). Based on theoretical frame on graph theory, the fragmentation algorithm on pair of vertices containing the largest fragments (called MaxF) are exemplified. The counting polynomials are used to enumerate number of all connected substructures and their sizes. For a general class of graphs called dendrimers general formulas giving counting polynomials are obtained and characterized using informational measures.

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References

- [1] S. D. Bolboacă and L. Jäntschi, *How Good the Characteristic Polynomial Can Be for Correlations?*, International Journal of Molecular Sciences, **8** (2007), 335-345. DOI [10.3390/i8040335](https://doi.org/10.3390/i8040335).
- [2] L. Boltzmann, *Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen*, Wiener Berichte, **66** (1872), 275-370. JFM [04.0566.01](https://doi.org/10.1515/JFM.1872.011).
- [3] M. V. Diudea, I. Gutman and L. Jäntschi, *Molecular Topology*, Nova Science Publishers, 2001, LoC [2001031282](https://www.loc.gov/loc/olc/2001031282).
- [4] M. V. Diudea and C. L. Nagy, *Counting polynomials on nanostructures. In: Periodic Nanostructures*. Series: Developments in Fullerene Science, **7** (2007), 69-114. DOI [10.1007/978-1-4020-6020-5_4](https://doi.org/10.1007/978-1-4020-6020-5_4).

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- [5] M. V. Diudea, A. E. Vizitiu and D. Janezic, *Cluj and related polynomials applied in correlating studies*, Journal of Chemical Information and Modeling, **47** (2007), 864-874. DOI [10.1021/ci600482j](https://doi.org/10.1021/ci600482j).
- [6] L. Jäntschi, S. D. Bolboacă and C. M. Furdui, *Characteristic and Counting Polynomials: Modelling Nonane Isomers Properties*, Molecular Simulation, **35** (2009), 220-227. DOI [10.1080/08927020802398892](https://doi.org/10.1080/08927020802398892).
- [7] L. Jäntschi and M. V. Diudea, *Subgraphs of pair vertices*, Journal of Mathematical Chemistry, **45** (2009), 364-371. MR2470467. Zbl [1171.05433](https://zbmath.org/?q=ser/1171.05433).
- [8] J. F. Ragot, *Counting Polynomials with Zeros of Given Multiplicities in Finite Fields*, Finite Fields and Their Applications, **5** (1999), 219-231. MR1702893. Zbl [1024.11076](https://zbmath.org/?q=ser/1024.11076).
- [9] A. Rényi, *On measures of information and entropy*, Proceedings of the 4th Berkeley Symposium on Mathematics, Statistics and Probability, **1** (1961), 547-561. MR0132570(24 #A2410). Zbl [0106.33001](https://zbmath.org/?q=ser/0106.33001).
- [10] C. E. Shannon, *A Mathematical Theory of Communication*, Bell System Technical Journal, **27**(1948), 379-423 and 623-656. MR0026286(10,133e). Zbl [1154.94303](https://zbmath.org/?q=ser/1154.94303).
- [11] E. H. Simpson, *Measurement of Diversity*, Nature **163** (1949), 688-688. Zbl [0032.03902](https://zbmath.org/?q=ser/0032.03902).
- [12] R. P. Stanley, *Enumerative Combinatorics (I and II)*, In: Cambridge Studies in Advanced Mathematics, **49** and **62**, 1997 and 1999. MR1442260(98a:05001) and MR1676282(2000k:05026). Zbl [0945.05006](https://zbmath.org/?q=ser/0945.05006) and Zbl [0978.05002](https://zbmath.org/?q=ser/0978.05002).

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