

The structural information content of chemical networks

Matthias DEHMER, Frank EMMERT-STREIB

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

References

1. Diudea, M.V., Gutman, I., Jäntschi, L. (2002) *Molecular Topology*. NOVA, New York
2. Harary, F. (1962) *SIAM Rev*, 4, pp. 202-210.
3. Sachs, H. (1964) *Publ. Math. (Debrecen)*, 11, pp. 119-134.
4. Trinajstić, N. (1992) *Chemical Graph Theory*, 1st Ed CRC Press
5. Gutman, I., Milun, M., Trinajstić, N. (1975) *MATCH Commun. Math. Comput. Chem*, 1, pp. 171-175.
6. Aihara, J.-I. A new definition of Dewar-type resonance energies (1976) *Journal of the American Chemical Society*, 98 (10), pp. 2750-2758.
7. Gutman, I., Milun, M., Trinajstić, N. Graph theory and molecular orbitals. 19. Nonparametric resonance energies of arbitrary conjugated systems (1977) *Journal of the American Chemical Society*, 99 (6), pp. 1692-1704.
8. Tang, A., Kiang, Y., Yan, G., Tai, S. (1986) *Graph Theoretical Molecular Orbitals*. Science Press, Beijing
9. Dwyer, P.S. (1951) *Linear Computations*. Wiley, N. Y
10. Fadeev, D.K., Sominskii, I.S. (1965) *Problems in Higher Algebra*. Freeman, San Francisco
11. Hosoya, H., Murakami, M., Gotoh, M. (1973) *Natl. Sci. Rept. Ochanomizu Univ*, 24, pp. 27-34.
12. Graham, R.L., Lovasz, L. (1978) *Adv. Math*, 29, pp. 60-88.
13. Diudea, M.V., Ivanciuc, O., Nikolić, S., Trinajstić, N. Matrices of reciprocal distance, polynomials and derived numbers (1997) *Match*, 35, pp. 41-64.
14. Ivanciuc, O., Diudea, M.V., Khadikar, P.V. New topological matrices and their polynomials (1998) *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, 37 (7), pp. 574-585.
15. Ivanciuc, O., Ivanciuc, T., Diudea, M.V. (1999) *Roum. Chem. Quart. Rev*, 7, pp. 41-67.
16. Hosoya, H. (1971) *Bull. Chem. Soc. Japan*, 44, pp. 2332-2339.
17. Hosoya, H. On some counting polynomials in chemistry (1988) *Discrete Applied Mathematics*, 19 (1-3), pp. 239-257.
18. Konstantinova, E.V., Diudea, M.V. The Wiener polynomial derivatives and other topological indices in chemical research (2000) *Croatica Chemica Acta*, 73 (2), pp. 383-403.
19. Gutman, I., Klavžar, S., Petkovšek, M., Žigert, P. On Hosoya polynomials of benzenoid graphs (2001) *Match*, 43, pp. 49-66.
20. Hosoya, H., Yamaguchi, T. (1975) *Tetrahedron Lett*, pp. 4659-4662.
21. Ohkami, N., Hosoya, H. Topological dependency of the aromatic sextets in polycyclic benzenoid hydrocarbons. Recursive relations of the sextet polynomial (1983) *Theoretica Chimica Acta*, 64 (3), pp. 153-170.
22. Ohkami, N., Motoyama, A., Yamaguchi, T., Hosoya, H. (1981) *Tetrahedron*, 37, pp. 1113-1122.
23. Hosoya, H. (1990) *Topics Curr. Chem*, 153, pp. 255-272.
24. Clar, E. (1964) *Polycyclic Hydrocarbons*. Acad. Press, London

25. Clar, E. (1972) *The Aromatic Sextet*. Wiley, New York
26. Gutman, I., Hosoya, H. (1990) *Z. Naturforsch*, 45 a, pp. 645-648.
27. Gutman, I. (1992) *MATCH Commun. Math. Chem*, 28, pp. 139-150.
28. Stevanović, D. (1998) *Graph Theory Notes New York*, 34, p. 3136.
29. Motoyama, A., Hosoya, H. King and domino polynomials for polyomino graphs (1976) *Journal of Mathematical Physics*, 18 (7), pp. 1485-1490.
30. Balasubramanian, K., Ramaraj, R. (1985) *J. Comput. Chem*, 6, pp. 447-454.
31. Farrell, E.J. (1978) *Canad. Math. Bull*, 2, pp. 35-46.
32. Farrell, E.J., De Matas, C.M. On star polynomials of complements of graphs (1988) *Arkiv för matematik*, 26 (1), pp. 185-190.
33. Farrell, E.J., De Matas, C. (1988) *Util. Math*, 33, pp. 33-45.
34. Diudea, M.V. Molecular topology. 16. Layer matrices in molecular graphs (1994) *Journal of Chemical Information and Computer Sciences*, 34 (5), pp. 1064-1071.
35. Diudea, M.V. (2002) *Studia Univ. Babeş-Bolyai Ser. Chemia*, 47, pp. 131-139.
36. Diudea, M.V. Hosoya polynomial in Tori (2002) *Match*, (45), pp. 109-122.
37. Diudea, M.V., Ursu, O. Layer matrices and distance property descriptors (2003) *Indian Journal of Chemistry - Section A Inorganic, Physical, Theoretical and Analytical Chemistry*, 42 (6), pp. 1283-1294.
38. Stefu, M., Diudea, M.V. (2005) *Nanostructures - Novel Architecture*, pp. 127-165. M. V. Diudea, Ed, Nova, New York
39. Ursu, O., Diudea, M.V. (2005) TOPOCLUJ software program Babeş-Bolyai University, Cluj, available at <http://chem.ubbcluj/~diudea>
40. John, P.E., Khadikar, P.V., Singh, J. J. *Math. Chem* DOI:10.1007/s10910-006-9100-2
41. John, P.E., Vizitiu, A.E., Cigher, S., Diudea, M.V. CI index in tubular nanostructures (2007) *Match*, 57 (2), pp. 479-484.
42. Klavžar, S. Some comments on Co graphs and CI index (2008) *Match*, 59 (1), pp. 217-222.
43. Ovchinnikov, S., arXiv (2007) 0704.0010v1 [math CO] 31 Mar
44. Djoković, D.Z. (1973) *J. Combin. Theory Ser. B*, 14, pp. 263-267.
45. Winkler, P.M. (1984) *Discrete Appl. Math*, 8, pp. 209-212.
46. Diudea, M.V., Vizitiu, A.E., Janežič, D. Cluj and related polynomials applied in correlating studies (2007) *Journal of Chemical Information and Modeling*, 47 (3), pp. 864-874.
47. Diudea, M.V., Cigher, S., Vizitiu, A.E., Ursu, O., John, P.E. Omega polynomial in tubular nanostructures (2006) *Croatica Chemica Acta*, 79 (3), pp. 445-448.
48. Vizitiu, A.E., Cigher, S., Diudea, M.V., Florescu, M.S. Omega polynomial in ((4,8)3) tubular nanostructures (2007) *Match*, 57 (2), pp. 457-462.
49. Diudea, M.V. (2006) *Carpath. J. Math*, 22, pp. 43-47.
50. Ashrafi, A.R., Manoochehrian, B., Yousefi-Azari, H. On the PI polynomial of a graph (2006) *Utilitas Mathematica*, 71, pp. 97-108.
51. Khadikar, P.V. (2000) *Nat. Acad. Sci. Letters*, 23, pp. 113-118.
52. Klavžar, S. On the PI index: PI-partitions and Cartesian product graphs (2007) *Match*, 57 (3), pp. 573-586.
53. Diudea, M.V., Nagy, C.L. (2007) *Periodic Nanostructures*. Springer
54. Diudea, M.V., Florescu, M.S., Khadikar, P.V. (2006) *Molecular Topology and Its Applications*. EFICON, Bucharest
55. M. V. Diudea, S. Cigher, A. E. Vizitiu, M. S. Florescu, and P. E. John, *J. Math. Chem.*, 2007, 44, 000-000.