

Sadhana polynomial in nano-dendrimers

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ABSTRACT.

Sadhana polynomial is defined on the ground of quasi orthogonal cut qoc strips in a graph $G = G(V, E)$. A qoc strip, defined with respect to any edge in G , represents the smallest subset of edges closed under taking opposite edges on faces. The first derivative, in $x = 1$, of Sadhana polynomial is a multiple of the number of edges in the graph. Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. In high generation dendrimers, it is difficult to calculate this polynomial. Thus, the composition of the global polynomial by monomeric contributions would facilitate the computation. Composition rule for in a family of nano-dendrimers, according to their topology, is derived.

REFERENCES

- [1] Ashrafi, A. R., Ghorbani M. and Jalali, M., *Computing Sadhana polynomial of V-phenylenic nanotubes and nanotori*, Indian J. Chem., **47A** (2008), 535-537
- [2] Ashrafi, A. R. and Mirzargar, M., *PI, Szeged and edge Szeged indices of an infinite family of nanostar dendrimers*, Indian J. Chem., **47A** (2008), 538-541
- [3] Aziz, S., Manikpuri, A. D., Khadikar, P. V., John, P. E., *Sadhana: A New Topological Index for Carbon Nanotubes(CNTs)*, J. Comput. Theor. NanoSci. **6** (2009), 1-3
- [4] Aziz, S., Khadikar, P. V. and John, P. E., *Sadhana Index(Sd) A Novel Graph Theoretical Descriptor for Quantative Structure-Property Relationship*, Natl. Acad. Sci. Lett., **32** (2009), 111-122
- [5] Bosman, A. W. and Meijer, E. W., *About Dendrimers: Structure, Physical Properties, and Applications*, Chem. Rev., **99** (1999), 1665-1688
- [6] Cigher, S., Diudea, M. V., *Omega Polynomial Counter*, "Babes-Bolyai" Univ., 2007; *Kekul Counter*, "Babes-Bolyai" Univ., 2008
- [7] Clar, E., *Polycyclic Hydrocarbons*, Acad. Press, London, 1964
- [8] Clar, E., *The Aromatic Sextet*, Wiley, New York, 1972
- [9] Diudea, M. V. and Katona, G., *Molecular topology of dendrimers*, in: G. A. Newkome, Ed., *Advan. Dendritic Macromol.*, **4**, (1999), 135-201
- [10] Diudea, M. V., Kacsó, I. E. and Minailiuc, O. M., *Y-Indices in Homogeneous Dendrimers*, MATCH Commun. Math. Comput. Chem. **28** (1992), 61-99
- [11] Diudea, M. V., *Orbital and wedgeal subgraph enumeration in dendrimers*, MATCH Commun. Math. Comput. Chem., **30** (1994), 79-91
- [12] Diudea, M. V., *Wiener index of dendrimers*, MATCH Commun. Math. Comput. Chem., **32** (1995), 71-83
- [13] Diudea M. V. and Parv, B., *Hyper-Wiener index of dendrimers*, J. Chem. Inf. Comput. Sci. **35** (1995), 1015-1018
- [14] Diudea, M. V., Katona, G. and Parv, B., *Delta number, Dde of dendrimers*, Croat. Chem. Acta **70** (1997), 509-517
- [15] Diudea, M. V., Kiss, A. A., Estrada, E. and Guevara, N., *Connectivity-, Wiener- and Harary-type indices of dendrimers*, Croat. Chem. Acta **73** (2000), 367-381
- [16] Diudea, M. V., Gutman, I. and Jantschi, L., *Molecular Topology*, NOVA, New York, 2002
- [17] Diudea, M. V., John, P. E., Graovac, A., Primorac, M. and Pisanski, T., *Leapfrog and related operations on toroidal fullerenes*, Croat. Chem. Acta **76** (2003), 153-159
- [18] Diudea, M. V., *Covering forms in nanostructures*, Forma (Tokyo) **19** (2004), 131-163
- [19] Diudea, M. V., Stefu, M., John, P. E. and Graovac, A., *Generalized operations on maps*, Croat. Chem. Acta **79** (2006), 355-362
- [20] Diudea, M. V., *Nanoporous carbon allotropes by septupling map operations*, J. Chem. Inf. Model. **45** (2005), 1002-1009
- [21] Diudea, M. V., *Omega Polynomial*, Carpath. J. Math. **22**, 2006, 43-47
- [22] Diudea, M. V., S. Cigher and P. E. John, *Omega and related counting polynomials*, MATCH Commun. Math. Comput. Chem. **60** (2008), 237-250
- [23] Diudea, M. V., Ed., *Nanostructure, Novel Architecture*, Nova, N. Y., 2005
- [24] Diudea, M. V. and Cs. Nagy, L., *Periodic nanostructures*, Springer, 2007.
- [25] Estrada, E., Guevara, N., Kiss, A. A., Motoc, F. and Diudea, M. V., *Connectivity indices of dendrimers*, Studia Univ. "Babes-Bolyai" **45** (2001), 71-80
- [26] M. V. Diudea, *Nanoporous carbon allotropes by septupling map operations*, J. Chem. Inf. Model., 2005, 45, 1002-1009.
- [27] Fowler P. W. and Pisanski, T., *Leapfrog Transformation and polyhedra of Clar type*, J. Chem. Soc. Faraday Trans. **90** (1994), 2865-2871
- [28] Fowler, P. W. and Manolopoulos, D. E., *An Atlas of Fullerenes*, Clarendon Press, Oxford, 1995
- [29] Fries, K. and Liebigs, J., *Über bicyclische verbindungen und ihren vergleich mit dem naphthalin*, III Mitteilung, Justus Liebigs Ann. Chem. **454**, 121-324
- [30] Gilles, E. R. and Frechet, J. M. J., *Dendrimers and dendritic polymers in drug delivery*, Drug Discovery Today, **10** (2005), 35-43
- [31] Harary, F., *Graph Theory*, Addison-Wesley, Reading, MA, 1969
- [32] Hawker, C. J. and Frechet, J. M. J., *Preparation of Polymers with Controlled Molecular Architecture. A New Convergent Approach to Dendritic Macromolecules*, J. Am. Chem. Soc. **112** (1990), 7638-7647
- [33] Khadikar, P. V., Agrawal, V. K. and Karmarkar, S., *Prediction of Lipophilicity of Polyacenes Using Quantitative Structure-Activity Relationships*, Bioorg. Med. Chem. **10** (2002), 3499-3507
- [34] Khadikar, P. V., Joshi, S., Bajaj, A. V. and Mandloi, D., *Correlations between the Benzene Character of Acenes or Helicenes and Simple Molecular Descriptors*, Bioorg. Med. Chem. Lett. **14** (2004), 1187- 1191
- [35] Khadikar, P. V., Singh, S., Jaiswal, M. and Mandoli, D., *Topological Estimation of Electronic Absorption Bands: Arene Absorption Spectra as a Tool for Modeling Their Toxicity Environmental Pollution*, Bioorg. Med. Chem. Lett. **14** (2004), 4795-4801
- [36] Khadikar, P. V., Singh, J. and Ingle, M., *Topological Estimation of Aromatic Stabilities of Polyacenes and Helicenes: Modeling of Resonance Energy and Benzene Chatacter*, J. Math. Chem. **42** (2007), 433-446

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- [36] Khadikar, P. V., Mandoli, D. and Karmakar, S., Sadhana(Sd): *A New Cyclic Index: QSPR/QSAR Studies of Linear Polyacenes*, *Bioinformatics Trends* **1** (2006), 51-63
- [37] Kim, Y. and Zimmerman, S. C., *Applications of Dendrimers in Bio-Organic Chemistry*, *Curr. Opin. Chem. Biol.* **2** (1998), 733-742
- [38] Newkome, G. R., Yao, Z.-Q., Baker, G. R. and Gupta, V. K., *Cascade molecules: a new approach to micelles. A [27] arborol*, *J. Org. Chem.* **50** (1985), 2003-2004
- [39] Newkome, G. R., Moorefield, C. N. and Voegtle, F., *Dendrimers and dendrons: Concepts, syntheses, applications*, Wiley-VCH, Weinheim, 2001
- [40] Newcome, G. R., Moorefield, C. N. and Vogtle, F., *Dendritic macromolecules: Concepts, syntheses, perspectives*, VCH: Weinheim, Germany, 1996
- [41] Smith, D. K. and Diederich, F., *Functional Dendrimers: Unique Biological Mimics*, *Chem. Eur. J.* **4** (1998), 1353-1361
- [42] Stefu, M., Diudea, M. V. and John, P. E., *Composite operations on maps*, *Studia Univ. "Babes-Bolyai"* **50** (2005), 165-174
- [43] Stiriba, S.-E., Frey, H. and Haag, R., *Dendritic polymers in biomedical applications: From potential to clinical use in diagnostics and therapy*, *Angew. Chem. Int. Ed.* **41** (2002), 1329-1334
- [44] Tomalia, D. A., Baker, H., Dewald, J. R., Hall, M., Kallos, G., Martin, S., Roeck, J., Ryder, J. and Smith, P., *A New Class of Polymers: Starburst-Dendritic Macromolecules*, *Polym. J. (Tokyo)* **17** (1985), 117-132
- [45] Tomalia, D. A., Naylor, A. M. and Goddard, W. A. I., *Starburst Dendrimers: Molecular- Level Control of Size, Shape, Surface Chemistry, Topology, and Flexibility from Atoms to Macroscopic Matter*, *Angew. Chem. Int. Ed.* **29** (1990), 138-175
- [46] Tomalia, D. A. and Frechet, J. M. J., *Discovery of dendrimers and dendritic polymers: A brief historical perspective*, *J. Polym. Sci., Part A: Polym. Chem.* **40** (2002), 2719-2728
- [47] Trinajstić, N., *Chemical Graph Theory*, (second ed.) CRC Press, Boca Raton, 1992

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