communications in mathematical
match
and in computer chemistry

32 (1995), 71-83

Molecular Topology 21. Wiener Index of Dendrimers

Mircea V. Diudea

Department of Chemistry, "Babes-Bolyai" University
3400 Cluj, Romania

Abstract: *General formulas for the calculation of the Wiener index, W, in regular and irregular dendrimers are proposed. They are derived on the basis of Wiener's algorithm [1] by using progressive vertex degrees and orbit numbers [2a] as parameters.*

1. Introduction.

The Wiener index, **W**, [1] is the sum of all topological distances in a graph, **G**. Hosoya [3] gave the actually well known relation for the calculation of this index, as the half sum of all entries in the distance **D** matrix

$$W = 1/2 \, \Sigma_i \Sigma_j \, d_{ij} \qquad (1)$$

Other formulas relate **W** with the distance sums, **DS** , [4,5] or with the distance degrees, $d^{(e)}{}_i$, [2b,6,7] in graph

$$W = 1/2 \, \Sigma_i DS_i = 1/2 \, \Sigma_i \Sigma_e \, (d^{(e)}{}_i * e) \qquad (2)$$

or also with the Laplacian eigenvalues, x_i [8-10]

$$W = N \sum_{i=2}^{N} 1 / x_i \qquad (3)$$

Several algorithms [9,11-21] for the evaluation of **W** were developed. Wiener itself calculated **W** [1] as the sum of contributions, $\mathbf{W_{(ij)}}$, of all edges in **G**, which, in acyclic structures, can be obtained by

$$\mathbf{W} = \Sigma_{(ij)}\ \mathbf{W_{(ij)}}\ = \Sigma_{(ij)}\ (\mathbf{N_i} * \mathbf{N_j}) \qquad (4)$$

where $\mathbf{N_i}$ and $\mathbf{N_j}$ denote the number of vertices in the fragments $\mathbf{f_i}$ and $\mathbf{f_j}$ resulted by cutting the edge **(ij)** (see also [5,14,15]).

Among the various modifications of **W** [7,14,22-47], the Schultz index [31-41] and the hyper-Wiener index [42-46] are the most important.

Schultz [33-39] has defined their molecular topological index, **MTI** , (known in the literature as the Schultz index) by

$$\mathbf{MTI} = \sum_{i=1}^{N} [\mathbf{v}(\mathbf{A} + \mathbf{D})]_i \qquad (5)$$

where **A** denotes the adjacency matrix and **v** is the vertex-valence vector. Gutman [32] decomposed the Schultz index as follows

$$\mathbf{MTI} = \sum_{i=1}^{N} (\mathbf{v}_i)^2 + 1/2 \sum_{i=1}^{N} \sum_{j=1}^{N} (\mathbf{v}_i + \mathbf{v}_j)\mathbf{D}_{ij} \qquad (6)$$

the second term being a vertex-valence-weighted Wiener index. Recall that Ivanciuc [27] and more recently Dobrynin [28] proposed invariants similar with the second term in eq **(6)**. The relatedness of **MTI** with **W** is quite obvious.

Randic' [42] introduced the so-called hyper-Wiener index, **R**, as

$$\mathbf{R} = \sum_{p}^{p \in G} \mathbf{N}_{1p} * \mathbf{N}_{2p} \qquad (7)$$

where N_{ip} denotes the number of vertices in the one of the two fragments which end a given path , **p**, in a tree. The product equals the number of all paths which include the selected path. The index **R** can be expressed as the half sum of the Wiener matrix entries, w_{ij} [43]

$$R = 1/2 \sum_i \sum_j w_{ij} \qquad (8)$$

Very recently, Klein, Lukovits and Gutman [46] extended the definition of **R** to account for cycle-containing structures :

$$R = 1/2 \sum_{i<j} (d_{ij}^2 + d_{ij}) = (D_2 + W)/2 \qquad (9)$$

The above formula relates the **R** index with the **W** index and the second moment of distance, D_2. A remark needs the Mohar index, $(TI)_1$, given by

$$(TI)_1 = 2 \log (M/N)W \qquad (10)$$

which is also related with **W** (**M** and **N** being the number of edges and vertices in graph, respectively) [8,10,47].

The Wiener index is "seen" as an approximate measure of the expansiveness of graphs (i.e. aliphatic hydrocarbons). It was the first structural parameter found to give good correlations with the thermodynamic properties of saturated hydrocarbons [1,48,49]. Since then, correlations of **W** with various physico-chemical [50,51] and biological [52-56] properties of molecules have been studied.

A recent review concerning the Wiener index is due to Gutman *et al.* [5b].

In this paper general formulas for evaluating the Wiener index in dendrimers are presented.

2. Wiener index in regular dendrimers

Dendrimers are hyperbranched molecules, synthesised by repeatable steps, either by adding branching blocks around a central *core* (thus obtaining a new, larger orbit or generation - the "divergent growth" approach [57-59]), or by building large branched blocks starting from the periphery and then attaching them to the core (the "convergent growth" approach [60-63]). These rigorously tailored structures are mainly organic compounds but inorganic components were also used [64-67].They show spherical shape, which can be functionalized[68-71], thus resulting in new interesting properties. Reviews in the field are available [72,73].

Some definitions in dendrimer topology are needed:

The vertices of a dendrimer, except the external end points, are considered as branching points. The number of edges emerging from each branching point is called progressive degree, **p** [2a] (i.e. the edges which enlarge the number of points of a newly added orbit). It equals to the classical degree, **k**, minus one: $\mathbf{p = k - 1}$. If all the branching points have the same degree, the dendrimer is called regular. Otherwise it is irregular.

A dendrimer is called *homogeneous* if all its radial chains (i.e. the chains starting from the core and ending in an external point) have the same length [72].

It is well known [74] that any tree has either a monocenter or a dicenter (i.e. two points joined by an edge). Accordingly, the dendrimers are said *monocentric* and *dicentric*, respectively. Examples are given in the FIGURE. The numbering of orbits (generations [2a,72]) starts with zero for the core and ends with **r**, which equals the radius of the dendrimer (i.e. the number of edges from the core to the external nodes).

Within this paper, a dendrimer is denoted by the following symbols:

$\mathbf{D_{r,p}}$ for monocentric, regular dendrimer, of generation **r** and progressive degree **p**;

$\mathbf{DD_{r,p}}$ for the corresponding dicentric regular dendrimer;

$\mathbf{ID_{r,p_s}}$ for monocentric, irregular dendrimer, of generation **r** and progressive degrees $\mathbf{p_s}$, varying along the radial chain from $\mathbf{p_0}$ to $\mathbf{p_{r-1}}$ ($\mathbf{p_r}$ equalling zero, by definition);

$\mathbf{IDD_{r,p_s}}$ for the corresponding irregular dicentric dendrimer.

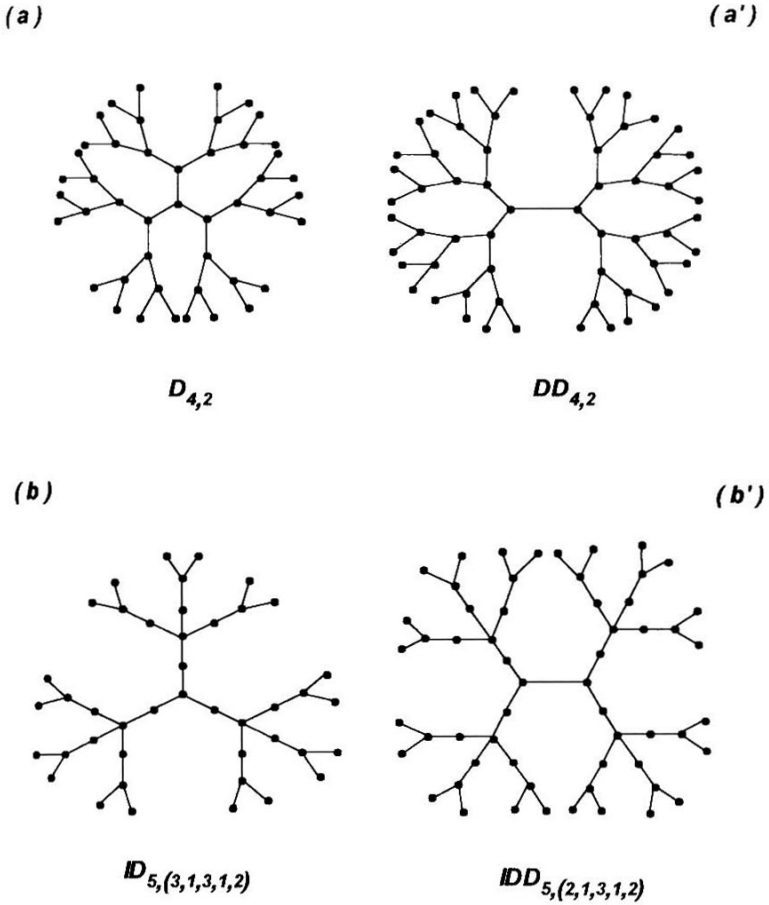

FIGURE. Regular (a) and irregular (b) monocentric and the corresponding dicentric, (a') and (b'), dendrimers

Notice that $p_0 = k_0$ for a monocentric irregular dendrimer, while for a dicentric one, $p_0 = k_0 - 1$, where k_0 and p_0 are the core classical and progressive degrees, respectively.

A *wedge* or a "subdendrimer" may result either by breaking an edge in a dendrimer, or by a step of "convergent" synthesis. If the cut edge ends at the core, the wedge is called *maximal*. The vertices of a wedge have the same degree as the corresponding ones in the whole dendrimer, except the cut point, whose degree is smaller by one.

Very recently, Gutman and a Chinese group [75] derived a special formula for the evaluation of the Wiener index in regular dendrimers. They used a combinatorial relationship applicable on any tree, which takes into account the decreasing effect of branching nodes on the magnitude of **W**, *versus* the path with the same number of vertices, **N**. However, the authors reported only formulas for monocentric regular (and the corresponding maximal wedge) dendrimers. In our notation, these are as follows:

$$W(D_{r,p}) = \{ [r(p+1)^3 - 2(r+1)(p+1)^2 + (p+1)]p^{2r} + 2(p+1)^2 p^r - (p+1)\} * (p-1)^{-3} \qquad (11)$$

$$W(Wed_{r,p}) = \{ [(r+2)(p+1) - 2(r+1)]p^{r+1} + [r(p+1) - 2(r+1)]p^{2r+2} \} * (p-1)^{-3} \qquad (12)$$

where $Wed_{r,p}$ means a dendrimer isomorphic with the maximal wedge in the dendrimer $D_{r,p}$.

We start with the observation that, in eq (4), $N_j = N - N_i$, so that a single parameter, N_i, needs to be calculated. The enumeration of points within the cut subgraphs f_i may be accomplished by the relationship

$$N_i = \sum_{s=i}^{r} p^{(r-s)} \qquad (13)$$

where r denotes the maximal orbit number in the dendrimer, s is the number of actual orbit and i is the number orbit of the cut point i. The number of all vertices in the dendrimer is given by

$$N(D_{r,p}) = (2-z)p^{r} + 2\sum_{s=0}^{r-1} p^{s} = 2\sum_{s=0}^{r} p^{s} - zp^{r} \qquad (14)$$

where $z = 1$ for a monocentric and $z = 0$ for a dicentric dendrimer, respectively.

Now, we can calculate $W_{(ij)}$ as well as their sum over all edges, cf. eq **(4)**, which is just the Wiener index, **W**.

Wiener index in regular dendrimers:

$$W(D_{r,p}) = (1-z)(N/2)^{2} + (p+1)^{z}(2p)^{(1-z)} * \sum_{s=1}^{r} p^{(s-1)}(N - N_s)N_s \qquad (15)$$

$$W(Orb(D_{r,p,s})) = (p+1)^{z}(2p)^{(1-z)} * p^{(s-1)}(N - N_s)N_s \qquad (16)$$

$$W(Wed_{r,p}) = \sum_{s=1}^{r} p^{(s-1)}(N - N_s)N_s \qquad (17)$$

$$W(Orb(Wed_{r,p,s})) = p^{(s-1)}(N - N_s)N_s \qquad (18)$$

$$W(D_{r,p}) = (1-z)(N/2)^{2} + (p+1)^{z}(2p)^{(1-z)} * W(Wed_{r,p}) \qquad (19)$$

$W(Orb(D_{r,p,s}))$ in eq **(16)** means the contribution of orbit **s** to the $W(D_{r,p})$ (i.e. the Wiener index for the whole dendrimer) whereas $W(Orb(Wed_{r,p,s}))$, in eq **(18)**, represents the corresponding contribution to the $W(Wed_{r,p})$. One can see that the global index $W(D_{r,p})$ can be expressed as a function of wedge contribution, $W(Wed_{r,p})$, eq **(19)**. The product

$(p+1)^z\ (2p)^{(1-z)}$ represents the "wedge factor", with the meaning of core progressive degree. The parameter z enables the use of eqs **(14)** through **(19)** both for monocentric and dicentric regular dendrimers.

By evaluating the sums in eq **(15)** results in two analytical expressions: one for $z = 1$, identical with eq **(11)** (i.e. the relationship for evaluating the Wiener index for the monocentric dendrimers) and another one for $z = 0$, which accounts for the Wiener index in dicentric dendrimers. The last one is as follows:

$$W(DD_{r,p};z=0) = [\ 4p^{(2r+2)}(p-1)r + (p-1)(p^{(r+1)}-1)^2 - 2p(p^r-1)(3p^{(r+1)}-1)](p-1)^{-3} \qquad (20)$$

The other relationships concerning the regular dendrimers are proposed as exercises for the reader.

3. Wiener index in irregular dendrimers

In irregular dendrimers, the power parameter p^s has to be transformed into the product $\prod_s p_s$, since in such dendrimers the progressive degree can change with the orbit, p_s being the progressive degree of orbit s. The population of the fragment f_i is now

$$N_i = 1 + \sum_{s=i}^{r} \prod_{v=i}^{s} p_v \qquad (21)$$

Thus, the formulas for evaluating W in irregular dendrimer are as follows:

Wiener index in irregular dendrimers:

$$N(ID_{r,p_s}) = (2-z)(1+\sum_{s=1}^{r}\prod_{v=0}^{s-1} p_v) \quad (22)$$

$$W(ID_{r,p_s}) = (1-z)(N/2)^2 + (2-z)\sum_{s=1}^{r}(\prod_{v=0}^{s-1} p_v)(N-N_s)N_s \quad (23)$$

$$W(Orb(ID_{r,p_s})) = (2-z)(\prod_{v=0}^{s-1} p_v)(N-N_s)N_s \quad (24)$$

$$W(IWed_{r,p_s}) = 1/p_0 \sum_{s=1}^{r}(\prod_{v=0}^{s-1} p_v)(N-N_s)N_s \quad (25)$$

$$W(Orb(IWed_{r,p_s})) = 1/p_0(\prod_{v=0}^{s-1} p_v)(N-N_s)N_s \quad (26)$$

$$W(ID_{r,p_s}) = (1-z)(N/2)^2 + (2-z)p_0 * W(IWed_{r,p_s}) \quad (27)$$

with $(2\text{-}z)p_0$ being the wedge factor and the remaining notations as in the case of regular dendrimers.

The Wiener index for a dendrimer isomorphic with the maximal wedge can be calculated either by the formula for $W(ID_{r,p_s})$, eq **(23)**, or by using that for $W(IWed_{r,p_s})$, (multiplied by p_0), eq **(25)**, mentioning that in both cases the orbit number **s** refers to the wedge orbits. As an example, the formula for the well known binary tree **(BT)** is given

$$W(BT) = \sum_{s=1}^{r}(\prod_{v=0}^{s-1} p_v)(N-N_s)N_s = \sum_{s=1}^{r} 2^s (N-N_s)N_s \quad (28)$$

where

$$N = \sum_{s=0}^{r} 2^s = 2^{(r+1)} - 1 \quad (29)$$

$$N_s = \sum_{v=s}^{r} 2^{(r-v)} = 2^{(r-s+1)} - 1 \qquad (30)$$

From eqs **(28)**, **(29)** and **(30)** , after a lengthy calculation, results in a formula which is identical with that obtained by the group of Gutman [75]:

$$W(BT) = (r+4)2^{(r+1)} + (r-2)2^{(2r+2)} \qquad (31)$$

A last remark: n-alkanes (P_N) can be viewed as regular dendrimers, with $p = 1$. In this case, eq **(15)** becomes

$$W(P_N) = (1-z)(N/2)^2 + 2\sum_{s=1}^{r}(N - N_s)N_s \qquad (32)$$

where

$$N_s = \sum_{s=i}^{r} p^{(r-s)} = r - s + 1 \qquad (33)$$

and taking into account that $r = (N - (2-z)) / 2$, eq **(32)** becomes

$$W(P_N) = (1-z)(N/2)^2 + 1/2\sum_{s=1}^{r}(N^2 - (2s-z)^2) \qquad (34)$$

The evaluation of sums leads to a formula which is independent of z

$$W(P_N) = 1/6(N^3 - N) = \binom{N+1}{3} \qquad (35)$$

and which is a well known result (see [75]).

Acknowledgements: Many thanks are expressed to Professor I. Gutman, Faculty of Science, University of Kragujevac, Yugoslavia, for reprints and very useful comments; I also thank to Dr. B. Pārv, Department of Mathematics, "Babes-Bolyai" University, Cluj, Romania, for computer assistance in verifying the equations.

References

[1] H. Wiener, *J.Am.Chem.Soc.*, **69** (1947) 17, 2636.

[2] (a) M.V. Diudea, *MATCH,* **30** (1994) 79 (Part 19); (b) M.V. Diudea, *Studia Univ. "Babes-Bolyai"*, **38** (1993) 3 (Part 20)..

[3] H. Hosoya, *Bull. Chem. Soc. Japan*, **44** (1971) 2332.

[4] O. Ivanciuc; T.S. Balaban; A.T. Balaban, *J. Math. Chem.*, **12** (1993) 21; 309.

[5] (a) I. Gutman; O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin 1986; (b) I. Gutman; Y.N Yeh; S.L. Lee; Y.L. Luo, *Indian J. Chem.,* **32A** (1993) 651; (c) I. Gutman; D.H. Rouvray, *Comput. Chem.*, **14** (1990) 29.

[6] H. Hosoya, *Discr. Appl. Math.*, **19** (1988) 239.

[7] M.V. Diudea, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 1064.

[8] N. Trinajstic'; D. Babic'; S. Nikolic'; D. Plavsic'; D. Amic'; Z. Mihalic', *J. Chem. Inf. Comput. Sci.*, **34** (1994) 368.

[9] I. Gutman, Shyi-Long Lee, Chih-Hung Chu, Yeung-Long Luo, *Indian J. Chem.*, **33A** (1994) 603.

[10] B. Mohar, D. Babić, N. Trinajstić, *J. Chem. Inf. Comput. Sci.*, **33** (1993) 153.

[11] S. Warshall, *J. Assoc. Comp. Math.*, **9** (1962) 11.

[12] B. Mohar; T. Pisanski, *J. Math. Chem.*, **2** (1988) 267.

[13] I. Lukovits, *Quant. Struct.-Act. Relat.*, **9** (1990) 227.

[14] I. Gutman, Graph Thepry Notes of New York, **27** (1994) 9 (New York Academy of Sciences)

[15] I. Gutman, *J. Mol. Struct.(Teochem)*, **285** (1993) 137.

[16] T. Pisanski, J. Žerovnik, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 395.

[17] I. Gutman, Yeong-Nan Yeh, Jiann-Cherng Chen, *Tamkang J. Math.*,. **25** (1994) 83.

[18] A. A. Dobrynin, *J. Math. Chem.*, **9** (1992) 239.

[19] M. Kunz, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 957.

[20] H. Hosoya, U. Nagashima, S. Hyugaji, *J. Chem. Inf. Comput. Sci.*, **33** (1993) 428.

[21] I. Gutman, *J. Serb. Chem. Soc.*, **58** (1993) 745.

[22] D. Bonchev; N. Trinajstic', *J. Chem. Phys.*, **67** (1977) 4517.

[23] B. Bogdanov; S. Nikolic'; N. Trinajstic', *J. Math. Chem.*, **5** (1990) 305.

[24] S.S. Tratch; M.I. Stankevitch; N.S. Zefirov, *Comput. Chem.*, **14** (1990) 29.

[25] A. Graovac; T. Pisanski, *J. Math. Chem.*, **8** (1991) 53.

[26] Z. Mihalic'; S. Nikolic'; N. Trinajstic, *J. Chem. Inf. Comput. Sci.*, **32** (1992) 28.

[27] O. Ivanciuc, *Rev. Roum. Chim.,* **34** (1989) 1361.

[28] A.A. Dobrynin; A.A. Kochetova, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 1082.

[29] D. Bonchev, A. T. Balaban, X. Liu, D. J. Klein, *Inter. J. Quantum Chem.*, **50** (1994) 1.

[30] D.J. Klein; M. Randic', *J. Math. Chem.,* **12** (1993) 81.

[31] D.J. Klein; Z. Mihalic'; D. Plavsic'; N. Trinajstic', *J. Chem. Inf. Comput. Sci.*, **32** (1992) 304.

[32] I. Gutman, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 1087.

[33] H.P. Schultz, *J. Chem. Inf. Comput. Sci.*, **29** (1989) 227.

[34] H.P. Schultz; E.B. Schultz; T.P. Schults, *J. Chem. Inf. Comput. Sci.*, **30** (1990) 27.

[35] H.P. Schultz; T.P. Schults, *J. Chem. Inf. Comput. Sci.*, **31** (1991) 144.

[36] H.P. Schultz; E.B. Schultz; T.P. Schults, *J. Chem. Inf. Comput. Sci.*, **32** (1992) 69.

[37] H.P. Schultz; T.P. Schults, *J. Chem. Inf. Comput. Sci.*, **32** (1992) 364.

[38] H.P. Schultz; T.P. Schults, *J. Chem. Inf. Comput. Sci.*, **33** (1993) 240.

[39] H.P. Schultz; E.B. Schultz; T.P. Schults, *J. Chem. Inf. Comput. Sci.*, **33** (1993) 863.

[40] H.P. Schultz; E.B. Schultz; T.P. Schults, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 1151.

[41] D. Plavšić, S. Nikolić, N. Trinajstić, *Croat. Chem. Acta* , **66** (1993) 345.

[42] M. Randic', *Chem. Phys. Lett.,* **211** (1993) 478.

[43] M. Randić, X. Guo, T. Oxley, H. Krishnapriyan, L. Nayor, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 361.

[44] I. Lukovits; W. Linert, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 899.

[45] I. Lukovits, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 1079.

[46] D.J. Klein; I. Lukovits; I. Gutman, *J. Chem. Inf. Comput. Sci.*, **35** (1995) 50.

[47] B. Mohar, *MATH./CHEM./COMP. 1988*; A. Graovac, Ed., Elsevier, Amsterdam, 1989; p. 1; *Graphs Comb.*, **7** (1991) 53.

[48] H. Wiener, *J. Chem. Phys.*, **15** (1947) 766.

[49] H. Wiener, *J. Phys. Chem.*, **52** (1948) 425, 1082.

[50] O. Mekenyan; D. Bonchev; N. Trinajstic', *Int. J. Quantum Chem.*, **18** (1980) 369.

[51] I. Lukovits, *Int. J.Quantum Chem.*, Quantum Biol.Symp., **19** (1992) 219.

[52] L.B. Kier; L.H. Hall, Molecular Connectivity in Chemistry and

Drug Research, (Academic Press, New York, 1976).

[53] S.C. Basak; L.J. Monsrud; M.E. Rosen; C.M. Frane; V.R. Magnuson, *Acta Pharm.Jugosl.*, **36** (1986) 81.

[54] I. Lukovits, *J. Chem. Soc., Perkin Trans.*, II, (1988) 1667.

[55] S. Nikolic'; M. Medic'-Sarc'; J. Matijevic'-Sosa, *Croat.Chem.Acta*, **66** (1993) 151.

[56] S. Mediratta, A. K. Madan, *J. Chem. Inf. Comput. Sci.*, **34** (1994) 867 .

[57] G.R. Newkome; G.R. Baker; M.J. Saunders; P.S. Russo; V.K. Gupta; Z.Q. Yao; J.E. Miller; K. Bouillon, *J.Chem.Soc., Chem.Commun.*, (1986) 752.

[58] A.M. Naylor; W.A. Goddard; G.E. Keifer; D.A. Tomalia, *J.Am.Chem.Soc.*, **111** (1989) 2339.

[59] A.B. Padies; H.K. Hall; D.A. Tomalia; J.R. McConnell, *J. Org. Chem.*, **52** (1989) 5305.

[60] C.J. Hawker; J.M. Frechet, *J. Am. Chem. Soc.*, **112** (1990) 7638.

[61] C.J. Hawker; R. Lee; J.M. Frechet, *J. Am. Chem. Soc.*, **113** (1991) 4583.

[62] K.L. Wooley; C.J. Hawker; J.M. Frechet, *J. Am. Chem. Soc.*, **113** (1991) 4252; *Angew. Chem.* **106** (1994) 123.

[63] D. Seebach; J.-M. Lapierre; K. Skobridis; G. Greiveldinger, *Angew. Chem.* **106** (1994) 457.

[64] L.J. Mathias; T.W. Carothers, *J. Am. Chem. Soc.*, **113** (1991) 4043.

[65] H. Uchida; Y. Kabe; K. Yoshino; A. Kawamata; S. Masamune, *J. Am. Chem. Soc.*, **113** (1991) 7077.

[66] S. Serroni; G. Denti; S. Campagna; A. Juris; M. Ciano; V. Balzani, *Angew. Chem., Int. Ed. Engl.* **31** (1992) 1493.

[67] G.R. Newkome; C.N. Moorefield; J.M. Keith; G.R. Baker; G.H. Escamilla, *Angew. Chem.* **106** (1994) 701.

[68] Z. Xu; J.S. Moore, *Angew. Chem.*, **105** (1993) 261; 1394.

[69] C. Worner; R. Mulhaupt, *Angew. Chem.*, **105** (1993) 1367.

[70] N. Launay; A.-M. Caminade; R. Lahana; J.-P. Majoral, *Angew. Chem.* **106** (1994) 1682.

[71] M.R. Bruce; W. Devonport; A.J. Moore, *Angew. Chem.* **106** (1994) 1862.

[72] D.A. Tomalia; A.M. Naylor; W.A. Goddard, *Angew.Chem., Int. Ed. Engl.*, **29** (1990) 138

[73] H.B. Mekelburger; W. Jaworek; F. Vogtle, *Angew.Chem., Int. Ed. Engl.*, **31** (1992) 1571

[74] F. Harary, Graph Theory, (Addison-Wesley, Reading, 1969).

[75] I. Gutman; Y.N. Yeh; S..L. Lee; J.C. Chen, *MATCH*, **30** (1994) 103