Theoretical Determination of Molecular Weight of AB₂ Dendrimers

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Abstract: The Molecular weight of any AB₂ type dendrimers were calculated by suggested theoretical equation. The results were compared with the data reported by others. It was found that there are no remarkable differences between the calculated and reported data.

Keywords: Dendrimer, Molecular weight, Lou-Mass number collection, Generations, PPI, AMAM.

Introduction

Dendrimers are highly branched macromolecules, obtained by an interactive sequence of reaction steps, having precisely defined molecular structures^{1,3,5}. These aesthetically appealing synthetic macromolecules distinguish themselves from normal polymers in two critical ways. Firstly, they are constructed from AB_n monomers which produce linear polymers. Thus, they contain hyper branched structures. Secondly, they are synthesized in an interactive fashion. The combination of these two features lead to a nonlinear, stepwise synthetic growth where in the number of monomer units incorporated in each successive interaction roughly doubles (AB₂) or triples AB₃.

That in the previous cycle, each repetition cycle lead to the addition of one more layer of branches which is a generation to the dendrimer from work. The generation number of the dendrimer is equal to the number of repetition cycles performed, and can be easily determined by counting the number of branch points as one proceeds from the core to the periphery^{2,4,6}.

In this paper, the molecular weight determination of various generations of an AB₂ dendrimer were calculated for four dendrimers: 1,2,4-triazole (TAZ), poly propylimine (PPI), 1,3,5-triazatriphosphinine derivative (MNBA), polyamidoamine (PAMAM) using the new suggested equation.

Results and Discussion

PPI is an AB₂ type polymer, in which the core is diaminobutane. The core has two active sites ($Z_0 = 2$), which can construct four branches for generation 1 (G1), eight branches for generation 2 (G2) and twelve branches for generation 3 (G3). Lou-Mass Number Collection (LMNC) can provide the number of branches in PPI dendrimer AB₂ for any generation where n is the number of each generation.

$$\text{LMNC} = 2 \times 2(2^n - 1) \quad (1)$$

One can generalize the above equation (1) to any type of dendrimer AB₂ by taking account of active positions (Z_0) of the core to the equation (1):

$$\text{LMNC} = 2Z_0(2^n - 1) \quad (2)$$

So, the number of the branches for any generations and for any type of dendrimer AB₂ (*i.e.* with $Z_0=1,2,3$ and 4) can be obtained from the equation (2) and could be illustrated as a mathematical collection (Lou-Mass Number Collection).

$$\text{LMNC}_{Z_0=1} = \{2, 6, 14, 30, 62, 126, \dots\}$$

$$\text{LMNC}_{Z_0=2} = \{4, 12, 28, 60, 124, 252, \dots\}$$

$$\text{LMNC}_{Z_0=3} = \{6, 18, 42, 90, 186, 378, \dots\}$$

$$\text{LMNC}_{Z_0=4} = \{8, 24, 56, 120, 248, 504, \dots\}$$

The results for 6 generations of the AB₂ dendrimer were outlined in Table 1.

Table 1. The number of branches for AB₂ dendrimers.

n	1	2	3	4	5	6
$\text{LMNC}_{Z_0=1}$	2	6	14	30	62	126
$\text{LMNC}_{Z_0=2}$	4	12	28	60	124	252
$\text{LMNC}_{Z_0=3}$	6	18	42	90	186	378
$\text{LMNC}_{Z_0=4}$	8	24	56	120	248	504

The molecular weight of a dendrimer is the sum of the molecular weight of branches and the molecular weight of core (M_{core}).

$$Mw_n = M_{\text{Core}} + (\text{LNC}_{Z_0}) M_r \quad (3)$$

$$Mw_n = M_{\text{Core}} + 2Z_0(2^n - 1) M_r \quad (4)$$

Molecular weight of the generation 1 and 3 of MNBA has reported⁷ which is 1052 and 5712 g mol⁻¹, respectively. By using the equation (3) and by replacing $Z_0 = 3$ for generation 1, the amount of molecular weight would be 1026 which has 1% of deviation from the experimental data.

$$M_r = 133, M_{\text{Core}} = 228$$

$$Mw_n = 228 + (6 \times 133) = 1026$$

Also the molecular weight for the generation 3 by using the equation (4) would be 5814 which has a 2% deviation.

$$Mw_n = 228 + 2 \times 3(2^3 - 1)133 = 228 + (42 \times 133) = 5814$$

The fundamental structure of a AB₂ dendrimers with different amount of Z_0 are outlined as below Figures 1-4.

$Z_0 = 1$
Figure 1.

$Z_0 = 2$
Figure 2.

$Z_0 = 3$
Figure 3.

$Z_0 = 4$
Figure 4.

The molecular structure of dendrimers TAZ, PPI, MNBA, PAMAM are in according to the structures in Figure 1- 4 respectively. Also, the same calculation of molecular weight was carried out for TAZ, PPI, MNBA and PAMAM and the results were summarized in Table 2.

Table 2. The reported and calculated molecular weights and percentage of error for TAZ, PPI, MNBA, PAMAM dendrimer

Dendrimer		Generation	Molecular Weight reported	Calculate Molecular Weight	Error percent,
TAZ $Z_0=1$	$M_{core}=174$	G_1	584 ^{13a}	584	0.0
	$M_i=205$	G_2	1404 ^{13a}	1312	7.0
	$M_{core}=159$	G_1	571 ^{13b}	569	0.35
	$M_i=205$				
PPI $Z_0=2$	$M_{core}=84$	G_1	316 ⁸	316	0.0
	$M_i=58$	G_2	773 ⁸	780	0.9
		G_3	1687 ⁸	1708	1.2
		G_4	3514 ⁸	3564	1.4
		G_5	7168 ⁸	7276	1.5
		G_5	7140 ¹²	7276	1.9
MNBA $Z_0=3$	$M_{core}=228$	G_1	1052 ⁷	1026	2.5
	$M_i=133$	G_3	5712 ⁷	5814	1.8
PAMAM $Z_0=4$	$M_{core}=516$	G_1	1430 ¹¹	1436	2.1
	$M_i=115$	G_3	6909 ¹¹	6956	0.7
		G_5	28824 ¹¹	29036	0.7
		G_6	58047 ¹¹	58476	0.74

As it is apparent from the table the inaccuracy of the molecular weight by comparing with those of Table 2 are trivial. It is interesting that with taking out of two continues LMNC_{Z₀} from the Table 1, one can find out the surface branch of the higher generation according to those reported by Newkome^{1,9,10}. The surface branches are shown in Table 3.

Table 3. The number of surface branches for AB₂ dendrimers.

Number of surface branch	Generation, n					
	1	2	3	4	5	6
$Z_0=1$	2	4	8	16	32	64
$Z_0=2$	4	8	16	32	64	128
$Z_0=3$	6	12	24	48	96	192
$Z_0=4$	8	16	32	64	128	256

Conclusions

The molecular weight of any AB₂ type dendrimers were calculated by suggested theoretical equation and compared to those reported. It was found that there are no remarkable differences between the calculated and reported data.

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