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Determination of molecular weight of poly (amidoamine) denderimer (PAMAM) by a new theoretical model

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ABSTRACT

The molecular weight determinations of various generations of AB_n dendrimer calculated for polyamidoamine (PAMAM) dendrimer by using our investigated equation.

Keyword: Molecular weight, Polyamidoamine, Denderimer (PAMAM), Diameter, AB_n

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INTRODUCTION

Dendrimers are highly branched macromolecules, obtained by an interactive sequence of reaction steps, having precisely defined molecular structures [1, 2]. They contain hyper branched structures and constructed form AB_2 monomer. The stepwise synthetic growth where in the number of monomer units incorporated in each successive interaction roughly doubles (AB_2) or triples AB_3 [1]. In the previous cycle, each repetition cycle lead to the addition of one more layer of branches which is a generation to the dendrimer [2-4]. The generation number of the dendrimer is equal to the number of repetition cycles performed [1, 2, 5] and can be easily determined by counting the number of branch points as one proceeds from the core to the periphery [2]. In contrast to traditional polymers, dendrimers are unique core–shell structures possessing three basic architectural components: a core (I), an interior of shells (generations) consisting of repeating branch-cell units (II) and terminal functional groups (the outer shell or periphery) (III) [4].

We have reported the molecular weight determination of various generations of an AB2 dendrimer for four denderimers: 1,2,4-triazole (TAZ) , poly propylimine (PPI), 1,3,5-triazatriphosphinine derivative (MNBA), polyamidoamine (PAMAM) [2]. In this paper the

molecular weight of various generations of AB_n dendrimer was calculated for polyamidoamine (PAMAM) dendrimer using our new investigated equation.

Data analysis:

The processes of branching can be done in two methods: $1 \rightarrow 2$ and $1 \rightarrow 3$[2, 4]. In the branching method ($1 \rightarrow 2$), the added monomer to the nucleus is activated in two points which is branched with two other branches. In the branching method ($1 \rightarrow 3$), the monomer which is connected to the nucleus has three active centers in order to be branched [4, 2].The PAMAM was created by method ($1 \rightarrow 2$). In the first generation it has 8 surface groups and in the other generations of 2,3,4,5,6 it has 16,32,64,128,256 surface groups, respectively. Naylor et al determined the molecular weight of the dendrimer with generation numbers 1 –10. This has been outlined in the table [3,4,5].

Table 1:The calculate molecular weight of PAMAM demdrimer and error values

Generation(G_n)	Ref.	Reported Molecular Weight(M_w)	percent error	Calculated Molecular weight
1	3	1430	12.9%	1614
2	3	3256	2.7%	3344
3	4	6909	0.2%	6926
4	5	14215	0.9%	14346
5	6	28826	3.1%	29715
6	4-6	58048	6.0%	61550
7	4-6	116493	9.4%	127492
8	4-6	233383	13.1%	264080
9	4-6	467126	17.1%	547003
10	4-6	934787	21.2%	1133033

The regression coefficient according to exponential equation (eq.) is 0.9995; M_w and n are molecular weight and generation numbers, respectively.

$$M_w = 779.31e^{0.7282\,n} \quad \text{(eq.)}$$

The molecular weight of the dendrimer in zero generation (n = 0), was calculated to be 779.31, which is the PAMAM molecular weight of the core. For generation one by substitution of n=1 in the equation, the molecular weight of PAMAM increases to 1614.

$M_w = 779.31 \times \exp(0.72821 \times 1) = 1614$

The percentage error between the experimental and theoretical value of the exponential model was obtained by the following equation:

$$\left| \frac{\text{Theoretical amount - experimental amount}}{\text{experimental amount}} \right| \times 100 = \text{percentage of error}$$

$$\left| \frac{1614 - 1430}{1430} \right| \times 100 = 12.9\%$$

So for the generation number 1 the percentage error is calculated (12.9%). Similar calculations was carried out for (n=2, 3...10). It is apparent that the inaccuracy of the molecular weights for the generation 1-6 is trivial (Table). The data has revealed that the average percentage of error was about 8.66. The variation of molecular weight against G_n is outlined in the Figure. For generations 1- 6 the molecular weight is linear, then onwards it is exponential. In generations 7 onwards there is significant rise in molecular weight.

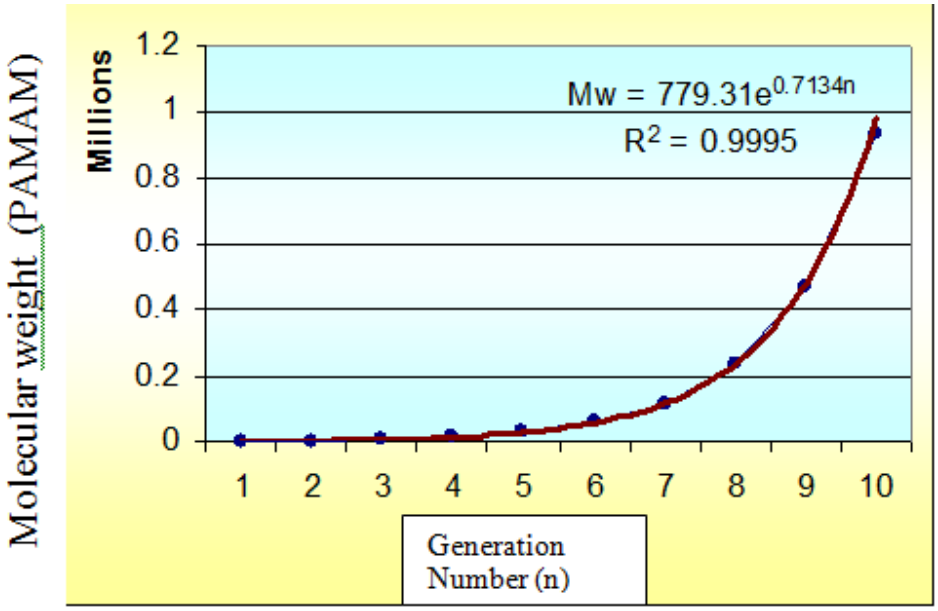

Figure : Diagram of exponential equations (eq.1)
Molecular weight of dendrimer at various generations.

CONCLUSION

The investigated equation provides a more accurate estimation of the molecular weight for various generations of AB_n PAMAM dendrimer, more specifically for generations 2-6. Research for a more accurate formula for determination of molecular weight is undergoing by our research group.

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