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DISPERSITY IN POLYMER SCIENCE

(IUPAC Recommendations 2009)

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Dispersity in polymer science

(IUPAC Recommendations 2009)

Abstract: This recommendation defines just three terms, viz., (1) molar-mass dispersity, relative-molecular-mass dispersity, or molecular-weight dispersity; (2) degree-of-polymerization dispersity; and (3) dispersity. "Dispersity" is a new word, coined to replace the misleading, but widely used term "polydispersity index" for $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$. The document, although brief, also has a broader significance in that it seeks to put the terminology describing dispersions of distributions of properties of polymeric (and non-polymeric) materials on an unambiguous and justifiable footing.

Keywords: dispersity; molar-mass dispersity; relative-molecular-mass dispersity; molecular-weight dispersity; degree-of-polymerization dispersity; polydispersity; polydispersity index; IUPAC Polymer Division.

INTRODUCTION

A dimensionless ratio of two average values of a property is widely used in polymer science as a characteristic of the dispersion, or spread, of the distribution of values of that property in a sample of polymer. In particular, the ratios $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$ are quantities commonly used to characterize the dispersions of distributions of molar masses and degrees of polymerization, respectively. However, they do not have satisfactory names and the present recommendation seeks to rectify this situation.

$\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$ are both often erroneously called "polydispersity index", although they are not indices and the term "polydispersity" is not a defined quantity. In addition, a polymer sample composed of a single macromolecular species should be called a "uniform polymer" and a polymer sample composed of macromolecular species of differing molar masses a "non-uniform polymer" [1]. It is preferable if such polymer samples are *not* called "monodisperse polymer" and "polydisperse polymer", respectively [1]. "Monodisperse" is a self-contradictory term, and "polydisperse" is tautologous.

The names proposed in this recommendation for $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$, are "molar-mass dispersity" and "degree-of-polymerization dispersity", respectively, with "relative-molecular-mass dispersity" and "molecular-weight dispersity" proposed as synonyms for molar-mass dispersity. "Dispersity" is a new word, coined to denote a measure of the dispersion of macromolecular species in a sample of polymer. The suffix "-ity" or "-ty" is described in dictionaries [2] as one used to form nouns describing quality, state of being or condition. In a scientific context, "-ity" is generally used to form nouns denoting the quality of a particular property, e.g., density, conductivity, resistivity, opacity, etc., in which the "quality" has a numerical value. Hence, "dispersity" is an appropriate word to describe a numerical attribute of the dispersion of a distribution.

The term "dispersity" is here limited to describing the dispersions of distributions of molar masses (or relative molecular masses, or molecular weights) and degrees of polymerization. With the use of suitable adjectives, it can easily be applied to distributions of other properties of samples of polymeric (and non-polymeric) materials, giving, for example, diffusion-coefficient dispersity and particle-diameter dispersity. Further applications and developments of the term will be the subject of future work. The immediate aim is to recommend satisfactory and widely acceptable names for $\bar{M}_w/\bar{M}_n$ and $\bar{X}_w/\bar{X}_n$. The general symbol $Đ$, pronounced "*D*-stroke", is introduced for dispersity to avoid confusion with the conventional use of D for diffusion coefficient.

DEFINITIONS

molar-mass dispersity, $Đ_M$
relative-molecular-mass dispersity
molecular-weight dispersity

Ratio of the mass-average molar mass, relative molecular mass, or molecular weight, $\bar{M}_w$, to the number-average molar mass, relative molar mass, or molecular weight, $\bar{M}_n$.

$$Đ_M = \bar{M}_w/\bar{M}_n$$

Note: Use of the term "polydispersity index" for $\bar{M}_w/\bar{M}_n$ or other terms involving the word "polydispersity" is strongly discouraged.

degree-of-polymerization dispersity, $Đ_X$

Ratio of the mass-average degree of polymerization, $\bar{X}_w$, to the number-average degree of polymerization, $\bar{X}_n$.

$$Đ_X = \bar{X}_w/\bar{X}_n$$

Note: Use of the term "polydispersity index" for $\bar{X}_w/\bar{X}_n$ or other terms involving the word "polydispersity" is strongly discouraged.

dispersity, $Đ$

Ratio of $\bar{M}_w$ to $\bar{M}_n$ or the ratio of $\bar{X}_w$ to $\bar{X}_n$ for a homopolymer or an alternating copolymer of sufficiently large molar mass, such that the effects of the distinct structures of the end-groups of the constituent macromolecules can be neglected, giving $\bar{X}_n$ directly proportional to $\bar{M}_n$, $\bar{X}_w$ directly proportional to $\bar{M}_w$ and $Đ_M = Đ_X = Đ$.

Note 1: Dispersity is a measure of the dispersion (or spread) of a molar-mass, relative-molecular-mass, molecular-weight, or degree-of-polymerization distribution. For a uniform polymer, $Đ = 1$; for a polymer of sufficiently high $\bar{X}_n$ having a Poisson distribution of molar masses, relative molecular masses, or molecular weights, $Đ \simeq 1$; and for a polymer of sufficiently high $\bar{X}_n$ having a most-probable distribution of molar masses, relative molecular masses, or molecular weights, $Đ \simeq 2$.

Note 2: For a copolymer that is not an alternating copolymer, $\bar{X}_n$ cannot be considered to be directly proportional to $\bar{M}_n$, nor $\bar{X}_w$ directly proportional to $\bar{M}_w$. It is then necessary to state whether $Đ_M$ or $Đ_X$ is being used.

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2. For example: *The Shorter Oxford English Dictionary*, 3rd ed., C. T. Onions, G. W. S. Friedrichsen (Eds.), Oxford University Press (1973); *The Pocket Oxford Dictionary of Current English*, 6th ed., J. B. Sykes (Ed.), Oxford University Press (1978).