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POLYMER DIVISION
SUB-COMMITTEE ON POLYMER TERMINOLOGY***DISPERSITY****(IUPAC Recommendation 2008)**

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Dispersity (IUPAC Recommendation 2008)

ABSTRACT

This recommendation defines just three terms, viz., molar-mass dispersity, degree-of-polymerization dispersity, and 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, degree-of-polymerization dispersity, polydispersity, polydispersity index.

PREAMBLE

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 characterise 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. ‘Dispersity’ is a new word, coined to denote a measure of the dispersion of macromolecular species in a sample of polymer. The suffix ‘-ity’ is described in dictionaries as one used ‘to form nouns of quality’. In a scientific context, that generally means 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 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 .

DEFINITIONS

1 molar-mass dispersity, D_M

Ratio of the mass-average molar mass, \bar{M}_w , to the number-average molar mass, \bar{M}_n .

$$D_M = \bar{M}_w / \bar{M}_n.$$

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

2 degree-of-polymerization dispersity, D_X

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

$$D_X = \bar{X}_w / \bar{X}_n.$$

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

3 dispersity, D

Ratio of \bar{M}_w to \bar{M}_n or the ratio of \bar{X}_w to \bar{X}_n for a homopolymer 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 $D_M = D_X = D$.

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

Note 2: For a 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 D_M or D_X is being used.

REFERENCE

1. *Compendium of Macromolecular Nomenclature*, W.V. Metanomski (ed.), Blackwell Scientific Publications, Oxford, 1991, Chapter 3.