



Nomenclature and Terminology for Dendrimers with Regular Dendrons and for Hyperbranched Polymers

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Nomenclature and Terminology for Dendrimers with Regular Dendrons and for Hyperbranched Polymers (Provisional Recommendations)

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Abstract: This document provides recommendations for (i) definitions of terms related to dendrimers with regular dendrons and to hyperbranched polymers and (ii) nomenclature for naming these complex compounds on the basis of structure-based nomenclature for regular and irregular organic polymers, including adjustments required for specifying dendritic and hyperbranched macromolecular structures. These recommendations and the examples deal with organic chemical structures only, but the general principles described in this document can be applied to inorganic and to hybrid organic-inorganic dendrimers and hyperbranched macromolecules as well.

Keywords: IUPAC Division of Chemical Nomenclature and Structure Representation; IUPAC Polymer Division; nomenclature recommendations; terminology recommendations; dendrimers; hyperbranched polymers; structure-based polymer names.

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DH-0 INTRODUCTION

Almost forty years ago the first examples of regularly branched compounds were synthesised which were, at that time, called "cascade molecules" [1]. A few years later their tree-like structure inspired others to introduce the name "arborol" for such compounds (which was derived from Latin arbor = tree) [2], while Tomalia et al. used the term "dendrimer", which is derived from the Greek words δένδρον (déndron = tree) and μέρος (méros = part), contained in "oligomeric nature" mentioned as the origin by the authors [3]. A thorough review by Tomalia [4] further publicised the term 'dendrimer', which then became widely used and generally accepted (Fig. 1).

Naming dendrimers by the rules of the systematic nomenclature of organic chemistry is in principle possible but, depending on their size and more so on the exact position of the senior functional group, would be cumbersome. So, a first alternative systematic approach to naming dendrimers was published by Newkome et al. in 1993 [5], which was based on the class name "cascade". This system was later revised and expanded by Vögtle et al. to cover also irregular and more complex dendritic structures [6]. They used the parent name "cascadane", while other name components described individual parts of the structure and their position.

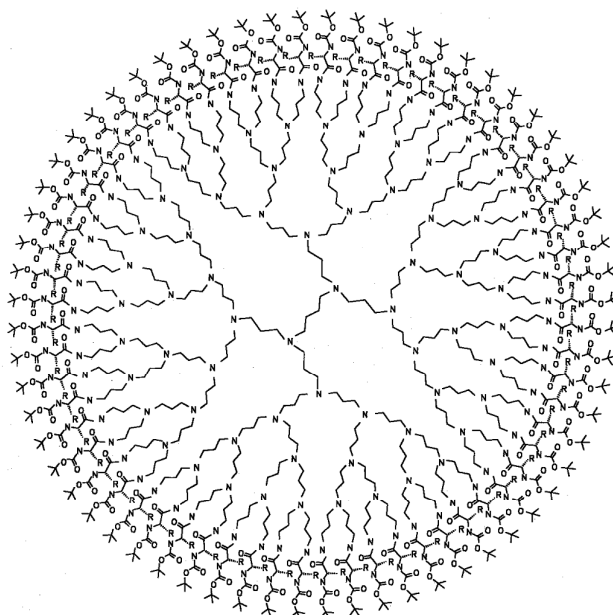


Fig. 1. Poly(propylene imine)-type dendrimer molecule with *tert*-butoxycarbonyl-protected phenylalanine end-groups ($R = -CH_2C_6H_5$). The H atoms are omitted for clarity [7].

Highly branched polymers that – at least in part – resemble dendrimers but in contrast to perfect or "almost perfect" dendrimers have a lower degree of branching are termed hyperbranched polymers (Fig. 2).

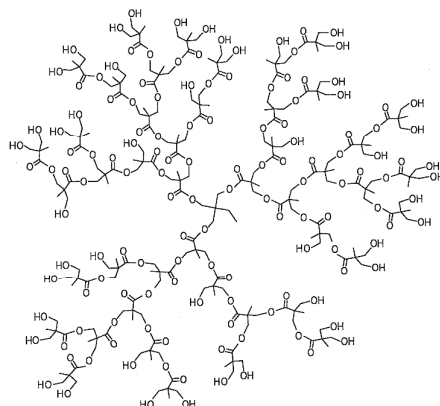


Fig. 2. Idealized representation of the hyperbranched aliphatic polyester molecule prepared by one-step bulk polyesterification of 3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic acid (AB_2 -type monomer) and 2-ethyl-2-(hydroxymethyl)propane-1,3-diol (B_3 -type monomer) in 45/1 mol ratio [8].

Both the regular repetition of structural units in dendrimer molecules and the molar mass of larger dendrimers make it suitable to use the principles of polymer nomenclature for naming them. Accordingly, the present document provides recommendations for naming dendrimers and hyperbranched polymers on the basis of structure-based nomenclature [9,10], including adjustments required for specifying dendritic and hyperbranched macromolecular structures. The present recommendations and the examples deal with organic chemical structures only. Nevertheless, the general principles described in this document can similarly be applied to inorganic and to hybrid inorganic-organic- dendrimers and hyperbranched polymers. The general principles of the underlying structure-based nomenclature of polymers [9–12] and of organic chemical compounds [13,14] are indispensable and will not be repeated here. The terminology section DH-1 gives definitions of the fundamental terms that are commonly used in the field of dendrimers and hyperbranched polymers and that are needed for understanding the rules given in the subsequent sections. The nomenclature sections DH-2 and DH-3 deal with dendrimers and hyperbranched macromolecular structures, respectively.

DH-1 DEFINITION OF TERMS RELATING TO DENDRIMERS AND HYPERBRANCHED POLYMERS

For ease of reference, the terms in this section are listed alphabetically and numbered sequentially. To assist the reader, within section DH-1, cross-references to terms also defined in this section are shown by using *italic* typeface.

The definition of a *dendrimer* is based on the definition of a *dendron*, which is a part of a molecule comprising exclusively *dendritic* and *terminal constitutional repeating units (CRUs)*. These units are defined on the basis of their *connectivity*, i.e. the number of other *CRUs* to which they are connected.

Those unfamiliar with the dendrimer and polymer domains should consider reading first the definitions of *macromolecule*, *oligomer molecule*, *chain*, *constitutional unit*, *constitutional repeating unit*, *connectivity*, *dendritic constitutional repeating unit*, *terminal constitutional repeating unit*, *dendron*, *dendrimer molecule* and *dendrimer*, in that order.

DH-1.1 branch [11,12]

Oligomeric or polymeric offshoot from a macromolecular *chain*.

DH-1.2 branch constitutional repeating unit

Constitutional repeating unit of connectivity three or more connected at least to three other constitutional repeating units.

Note 1: In addition, a branch constitutional repeating unit may also be connected to one or more end-groups.

DH-1.3 branch point [11,12]

Point on a *chain* at which a *branch* is attached.

DH-1.4 chain [11,12]

Whole or part of a *macromolecule*, an *oligomer molecule*, or a block, comprising a linear or branched sequence of *constitutional units* between two boundary *constitutional units*, each of which may be either an *end-group*, a *branch point* or an otherwise-designated characteristic feature of the *macromolecule*.

Note 1: Except in linear single-strand *macromolecules*, the definition of a *chain* may be somewhat arbitrary.

Note 2: See additional notes in refs [11,12].

**DH-1.5 connectivity (of a constitutional unit)
recommended symbol *c***

Number of covalent bonds emanating from a *constitutional unit*.

Note 1: For the purpose of determining connectivity a multiple bond is treated as one bond.

Note 2: In most cases, the connectivity of an end-group is 1. In some exceptional cases it can be higher, for instance when two hydroxy end-groups are modified into an acetal group.

DH-1.6 constitutional unit (CU) [11,12]

Atom or group of atoms (with pendant atoms or groups, if any) comprising a part of the essential structure of a *macromolecule*, an oligomer molecule, a block, or a chain.

DH-1.7 constitutional repeating unit (CRU) [11,12]

Smallest *constitutional unit*, the repetition of which constitutes a regular macromolecule, a regular oligomer molecule, a regular block, or a regular chain.

DH-1.8 core unit

Constitutional unit in a dendrimer molecule, from which the dendron(s) emanate(s).

- Note 1:* An example of a core unit in a dendrimer molecule is given in Fig. 3.
- Note 2:* The structure of the core unit may be identical to that of the *constitutional repeating units* (See Example 6 in DH-2.10).
- Note 3:* Occasionally, a dendrimer molecule may consist of two dendrons directly connected together (see also DH-1.11).
- Note 4:* In a hyperbranched macromolecule obtained by the AB_x -type monomer + B_y -type monomer polycondensation approach, where A and B refer to mutually reactive groups, the terms *core molecule* (not acceptable) and *core unit* refer to the B_y -type unit, even though the structure of the macromolecule does not comprise *dendrons*. See Fig. 2 for the example of a hyperbranched molecule of this type.

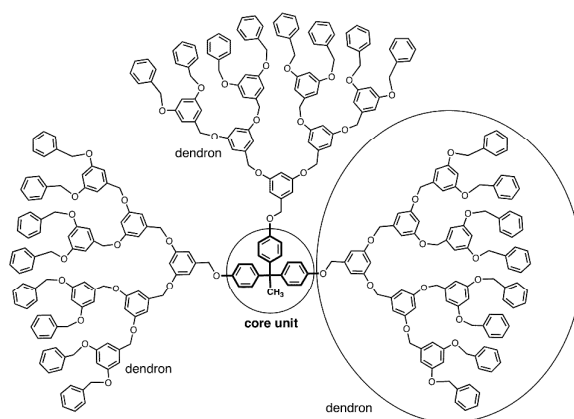


Fig. 3. Representation of a regular dendrimer molecule [15], highlighting the core unit and the dendrons.

DH-1.9 degree of branching
recommended symbol D_{br}

Parameter characterizing the branched architecture of a *hyperbranched polymer*, which is equal to unity for a polymer that contains no *linear* or *semi-dendritic constitutional repeating unit* and to 0 for a polymer that contains no *dendritic* or *semi-dendritic constitutional repeating unit*.

- Note 1:* Several definitions of the degree of branching have been proposed for *hyperbranched polymers* obtained by polycondensation of AB_2 -type monomers [16,17] and for those obtained by polycondensation of more complex monomer systems [17–20].
- Note 2:* The degree of branching of a *dendrimer* is equal to one. However, a polymer with the degree of branching equal to one is not necessarily a *dendrimer*. It can be a hyperbranched polymer, since the degree of branching does not per se take into account the regularity and symmetry of the molecules that compose it.
- Note 3:* The degree of branching of a linear polymer is equal to 0.

DH-1.10 dendrimer

Substance composed of identical *dendrimer molecules*.

DH-1.11 dendrimer molecule

Molecule consisting of one or more *dendrons* emanating from a single *constitutional unit*.

Note 1: See also DH-1.8.

Note 2: An example of dendrimer molecule is given in Fig. 3.

Note 3: Occasionally, a dendrimer molecule may consist of two *dendrons* directly connected together.

DH-1.12 dendritic block macromolecule

Block *macromolecule* in which at least one block is a *dendron*.

Note 1: See Examples 15 and 16 in DH-2.14.

Note 2: See the definition of a block macromolecule in refs [11,12].

DH-1.13 dendritic constitutional repeating unit

Constitutional repeating unit of connectivity $c \geq 3$ connected to c other *constitutional repeating units*.

Note 1: See Figs. 4 and 6.

Note 2: A dendritic constitutional repeating unit may be connected to one or more other *constitutional repeating units* via a *junction unit*.

Note 3: Dendritic constitutional repeating units belong to the class of *branch constitutional repeating units*.

DH-1.14 dendritic graft macromolecule

Graft macromolecule in which at least one of the grafts contains a *dendron*.

Note 1: See Examples 17 and 18 in DH-2.15.

Note 2: See the definition of a graft *macromolecule* in refs [11,12].

Note 3: A *dendritic graft macromolecule* is sometimes referred to as a *dendronised macromolecule*.

DH-1.15 dendritic macromolecule

Macromolecule containing at least one *dendron*.

DH-1.16 dendritic polymer

Substance composed of *dendritic macromolecules*.

Note: This definition differs from the definition of ‘dendritic polymer class’ in ref [21].

DH-1.17 dendron

Part of a molecule with only one free valence, comprising exclusively *dendritic* and *terminal constitutional repeating units* and in which each path from the free valence to any end-group comprises the same number of *constitutional repeating units*.

Note 1: For the purpose of determining the nature of *constitutional repeating units* the free valence is treated as a connection to a CRU.

Note 2: A *dendrimer molecule* comprising only one *dendron* is sometimes referred to as dendron, monodendron or functionalised dendron. The use of the terms ‘dendron’ or ‘monodendron’ in the meaning of molecule or substance is no longer acceptable. See also DH-1.11.

Note 3: In a *dendron*, macrocycles of *constitutional units* are absent (See Fig. 4).

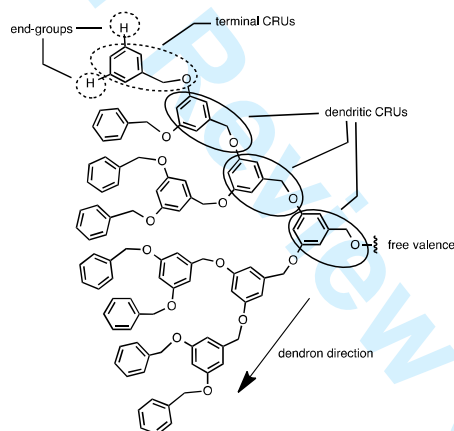


Fig. 4. Representation of a regular dendron, highlighting *dendritic constitutional repeating units*, *terminal constitutional repeating units*, end-groups, the *dendron direction* and the free valence. The preferred *constitutional repeating unit* is chosen according to rule DH-2.2.

DH-1.18 dendron direction

For a *constitutional repeating unit* of a *dendron*, the direction from the free valence to the end-groups.

Note: See Fig. 4.

DH-1.19 end-group [11,12]

Constitutional unit that is an extremity of a *macromolecule* or *oligomer molecule*.

Note: An *end-group* is attached to only one *constitutional unit* of a *macromolecule* or *oligomer molecule* (See Figs. 4–6).

DH-1.20 focal unit

Core unit of a dendrimer molecule that comprises only one dendron

DH-1.21 generation (in a dendron)

Set of constitutional repeating units separated from the free valence of a dendron by the same number of constitutional repeating units.

Note: Generations are numbered consecutively starting from the constitutional repeating unit bearing the free valence (See Fig. 5).

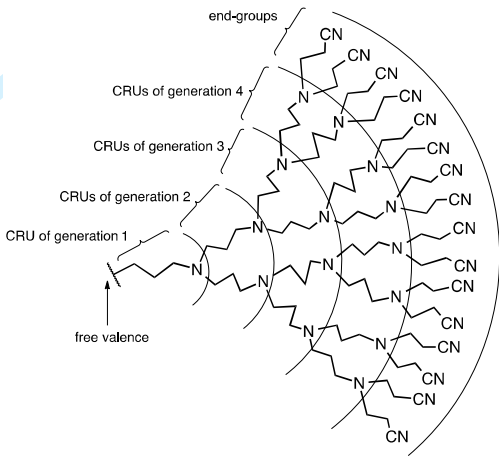


Fig. 5. Representation of a four-generation dendron, highlighting constitutional repeating units of generations 1 to 4 and the end-groups. The preferred constitutional repeating unit is chosen according to rule DH-2.2.

DH-1.22 hyperbranched macromolecule

Highly branched macromolecule, the constitutional repeating units of which are in substantial part branch constitutional repeating units and terminal constitutional repeating units.

Note 1: Hyperbranched macromolecules, unlike dendrimer molecules, usually comprise a number of randomly distributed linear constitutional repeating units (see Fig. 6).

Note 2: For the purpose of determining the type of constitutional repeating units (dendritic, semi-dendritic, terminal or linear CRUs) in a hyperbranched macromolecule, the core unit should be treated as a CRU.

DH-1.23 hyperbranched oligomer

Substance composed of hyperbranched oligomer molecules.

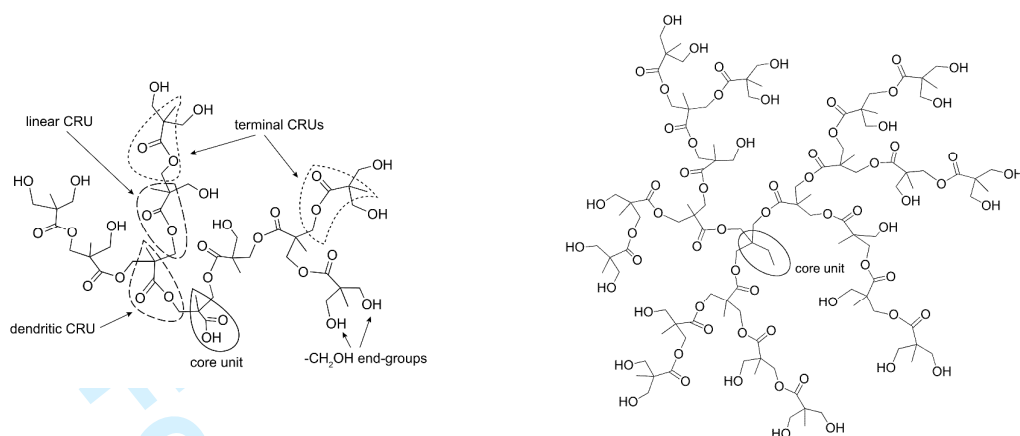


Fig. 6. Representation of hyperbranched molecules with a *core unit*. *Terminal, linear and dendritic constitutional repeating units, end-groups* and the *core unit* are circled. The preferred *constitutional repeating unit* is chosen according to rule DH-2.2.

DH-1.24 hyperbranched oligomer molecule

Highly branched *oligomer molecule*, the *constitutional repeating units* of which are in substantial part *branch constitutional repeating units* and *terminal constitutional repeating units*.

Note: See also DH-1.22, Notes 1 and 2.

DH-1.25 hyperbranched polymer

Substance composed of *hyperbranched macromolecules*.

Note 1: The term ‘dendrigrift’ is sometimes used for hyperbranched polymers of low molar-mass-dispersity. The use of ‘dendrigrift’ is discouraged.

Note 2: The present definition differs from the definition in the *Glossary of Class Names of Polymers* [21].

DH-1.26 irregular dendrimer

Substance composed of *irregular dendrimer molecules*.

DH-1.27 irregular macromolecule [11,12]

Macromolecule, the structure of which essentially comprises the repetition of more than one type of *constitutional unit*, or a *macromolecule* the structure of which comprises constitutional units not all connected identically with respect to directional sense.

DH-1.28 irregular dendrimer molecule

Dendrimer molecule that contains either different types of *regular dendrons* or at least one *irregular dendron*.

DH-1.29 irregular dendron

Dendron composed of either different types of *constitutional units*, different types of end-groups or any combination of these.

DH-1.30 linear constitutional repeating unit

Constitutional repeating unit connected to exactly two other *constitutional repeating units*.

Note 1: See Fig. 6.

Note 2: A *linear constitutional repeating unit* may be connected to one or more end-groups.

Note 3: *End-groups* attached to non-terminal *constitutional repeating units* are sometimes termed side groups. The use of the term side groups in this meaning is discouraged.

**DH-1.31 macromolecule [11,12]
polymer molecule**

Molecule of high relative molecular mass, the structure of which essentially comprises the multiple repetition of units derived, actually or conceptually, from molecules of low relative molecular mass.

Note 1: In many cases, especially for synthetic polymers, a molecule can be regarded as having a high relative molecular mass if the addition or removal of one or a few of the units has a negligible effect on the molecular properties. This statement fails in the case of certain properties of macromolecules which may be critically dependent on fine details of the molecular structure, e.g., the enzymatic properties of polypeptides.

Note 2: See additional notes in the original references.

**DH-1.32 number of generations (of a dendron)
recommended symbol: G**

Number of *constitutional repeating units* on the path from the free valence to any end-group of a *dendron*.

Note: The *number of generations* G is a cardinal number. A dendron with $G = n$ generations of constitutional repeating units should be called n generation dendron. The terms dendron of n^{th} generation or n^{th} generation dendron are no longer acceptable.

**DH-1.33 number of generations (of a regular dendrimer molecule)
recommended symbol: G**

Number of generation of the *dendrons* of a *regular dendrimer molecule*.

Note: See DH-1.32.

DH-1.34 number of pseudo-generations (of a hyperbranched polymer)

Number of generations of the hypothetical *dendrimer molecule* that would present the same ratio of constitutional repeating units to core unit.

Note 1: The number of pseudo-generations can be a decimal number, while the *number of generations* of a *dendrimer molecule* is an integer.

Note 2: In *hyperbranched polymers* obtained by the AB_x-type monomer + B_y-type monomer polycondensation approach, where A and B represent mutually reactive groups, the number of pseudo-generations *n* can be calculated by solving the equation:

$$r = y(x^n - 1)/(x - 1),$$

where *r* is the mol ratio of AB_x-type monomer per B_y-type monomer molecules (*core unit*). See Fig. 2 for an example of AB₂ and B₃-type monomers (*x* = 2 and *y* = 3).

Note 3: The use of the terms *generation* and *number of generations* for a *hyperbranched polymer* is no longer acceptable.

DH-1.35 oligomer [11,12]

Substance composed of *oligomer molecules*.

DH-1.36 oligomer molecule [11,12]

Molecule of intermediate relative molecular mass, the structure of which essentially comprises a small plurality of units derived, actually or conceptually, from molecules of lower relative molecular mass.

Note 1: A molecule is regarded as having an intermediate relative molecular mass if it has properties which do vary significantly with the removal of one or a few of the units.

Note 2: See additional notes in the original references

DH-1.37 polymer [11,12]

Substance composed of *macromolecules*.

DH-1.38 regular dendrimer

Substance composed of *regular dendrimer molecules*.

DH-1.39 regular dendrimer molecule

Dendrimer molecule comprising only identical *regular dendrons*.

Note: A *dendrimer* comprising only one *dendron* is a *regular dendrimer molecule*.

DH-1.40 regular dendron

Dendron composed of only one type of *constitutional repeating units* and of only one type of end-groups.

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DH-1.41 regular macromolecule [11,12]

Macromolecule, the structure of which essentially comprises the repetition of a single *constitutional unit* with all units connected identically with respect to directional sense.

DH-1.42 semi-dendritic constitutional repeating unit

Constitutional repeating unit of connectivity $c \geq 4$ connected to more than 2 but less than c other *constitutional repeating units*.

DH-1.43 terminal constitutional repeating unit

Constitutional repeating unit connected to only one other *constitutional repeating unit*.

- Note 1:* See Figs. 4 and 6.
- Note 2:* A terminal constitutional repeating unit may be connected to one or more end-groups

DH-2 NOMENCLATURE FOR DENDRIMERS

DH-2.0 General principles

Dendrimers can be named in two ways:

- by a form of organic chemistry multiplicative nomenclature [14] in which the core unit is a multivalent substituent and dendrons are multiple parent structures,
- by a form of organic chemistry substitutive nomenclature [14] in which the core unit is chosen as parent structure and dendrons are attached to it.

These two naming systems are extensions of existing polymer nomenclature rules for star polymers (ref. [12], rules 21 and 22, p. 294-5).

DH-2.1 Choice of multiplicative vs substitutive dendrimer nomenclature

DH-2.1.1 Multiplicative dendrimer nomenclature is preferred for most regular dendrimers, i.e.:

- regular dendrimers with a monovalent core unit.
- regular dendrimers with a multivalent simple core unit, i.e. a core unit consisting of a simple multiplicative component (e.g. $-\text{O}-$, $-\text{CH}_2-$, $-\text{N}<$, benzene-1,3,5-triyl, $-\text{CH}_2-\text{CH}_2-$), which may be substituted (e.g. $-\text{CH}(\text{CH}_3)-\text{CH}_2-$).
- regular dendrimers with a multivalent multipart symmetrical core unit, i.e. a core unit composed of concatenated simple multiplicative components (e.g. $-\text{CH}_2-\text{O}-\text{CH}_2-$, $\text{N}(\text{CH}_2-\text{CH}_2-)_3$). Substitution is allowed provided that the sequence of component units, starting from the central one, is identical in each of the branches.

Note: DH-2.1.1 essentially applies to dendrimers the general principles of organic chemistry multiplicative nomenclature, as detailed in ref. [14], § P-15.3.

DH-2.1.2 Multiplicative dendrimer nomenclature cannot be applied to regular dendrimers with multipart unsymmetrical core units, to regular dendrimers with unsymmetrical core units having different types of bonds (single/multiple), to regular dendrimers with symmetrical multipart core units composed of unsymmetrically substituted component units or to irregular dendrimers.

DH-2.1.3 Substitutive dendrimer nomenclature can be applied to any type of dendrimer or dendritic polymer and is the only one allowed for dendrimers of types other than those specified in DH-2.1.1.

Note: In dendrimer substitutive nomenclature, the core unit is always the parent structure.

DH-2.1.4 Naming a dendrimer by either type of nomenclature comprises the following steps:

- identification of the overall structure of dendrimer molecule: dendrons and core unit,
- choice of the preferred CRU(s),
- choice of the preferred end-group(s),
- choice of the preferred core unit and determination of its type (symmetrical or not, substituted or not),
- determination of the dendrimer type (regular, irregular) and of the number of generations of dendrons,
- naming the dendron(s),
- naming the dendrimer using multiplicative or substitutive nomenclature, depending on the core unit and dendrimer types.

DH-2.2 Choice of the preferred constitutional repeating unit (CRU) of a dendron

The preferred constitutional repeating unit of a dendron is chosen in such a way that the branch points be at its end in the dendron direction.

Note: Dendron direction is defined in DH-1.18.

DH-2.3 Choice of the preferred end-groups of a dendron

After the preferred constitutional repeating unit of a dendron has been defined, the preferred end-groups are chosen to maximize the number of generations of the dendron.

DH-2.4 Choice of the preferred core unit of a dendrimer molecule

After the preferred constitutional repeating unit and the preferred end-groups of the dendrons of a dendrimer have been defined, the preferred core unit is chosen to maximize the number of generations of the dendrons.

DH-2.5 Naming the preferred constitutional repeating unit (CRU) of a dendron

DH-2.5.1 The preferred constitutional repeating unit is named according to polymer nomenclature rules [12], by citing consecutively concatenated components in the dendron direction, the branch component being named last.

Note 1: Dendron direction is defined in DH-1.18

Note 2: Polymer nomenclature includes the following differences from organic chemistry nomenclature [22]:

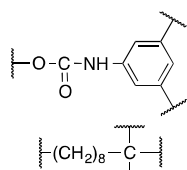
- ethylene is used as preferred name for $-\text{CH}_2-\text{CH}_2-$ instead of ethane-1,2-diyl [22,23].
- pendant groups, i.e. groups of atoms that are not part of the main chain, must be regarded as substituents, e.g. in a polymer chain, $-\text{CH}(\text{CH}_3)-\text{CH}_2-$ is 1-methylethylene, not propane-1,2-diyl.

DH-2.5.2 In a component of a dendrimer CRU, the lowest locant is assigned to the atom that is closest to the dendron free valence, except when the component has a fixed numbering. Atoms are numbered and cited in ascending order in the dendron direction.

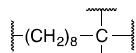
DH-2.5.3 The name of the preferred CRU remains the same in dendrimer multiplicative and substitutive nomenclature, i.e. it is not reversed when dendrons are regarded as substituents (see DH-2.9.2).

DH-2.5.4 Examples of CRU names

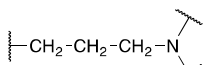
In the following table, the dendron direction is from left to right.



oxycarbonylazanediylbenzene-1,3,5-triyl
Locants are numbered and cited in the dendron direction.

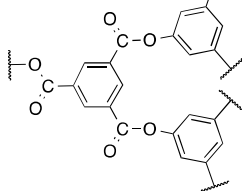


nonane-1,9,9,9-tetrayl
Branch point is numbered last in the dendron direction.

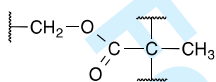


propane-1,3-diynitrile

Locants are numbered and cited in the dendron direction (1→3).

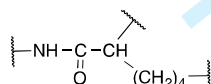


oxycarbonylbenzene-1,3,5-triylbis(carbonyloxybenzene-1,3,5-triyl).



methyleneoxy(2-methyl-1-oxoethane-1,2,2-triyl)

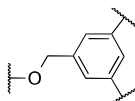
Branch point is numbered and cited last (locant 2). The oxo-substituted carbon (locant 1) is cited after methyl, in alphabetic order. According to polymer nomenclature, the branch component should not be named 1-oxopropane-1,2,2-triyl, since the methyl group is a substituent of the main chain.



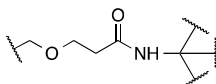
azanediyl(1-oxohexane-1,2,6-triyl)



oxy(methylsilanetriyl)



oxymethylenebenzene-1,3,5-triyl



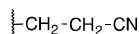
methyleneoxy(3-oxopropane-1,3-diyl)azanediylmethanetetrayl

The oxo substituent is on the last carbon of propane-1,3-diyl component, according to the dendron direction.

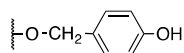
DH-2.6 Naming the end-groups

DH-2.6.1 The end-groups are named substitutively, according to organic chemistry nomenclature rules [14].

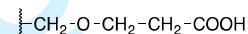
DH-2.6.2 Examples:



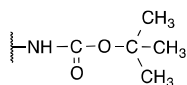
2-cyanoethyl



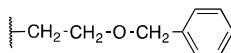
[4-hydroxyphenyl)methyl]oxy



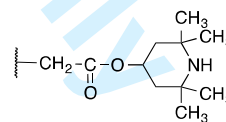
(2-carboxyethoxy)methyl



(tert-butoxycarbonyl)amino



2-(benzyloxy)ethyl



2-oxo-2-[(2,2,6,6-tetramethylpiperidin-4-yl)oxy]ethyl

DH-2.7 Naming the preferred core unit of a dendrimer molecule in multiplicative nomenclature

DH-2.7.1 In dendrimer multiplicative nomenclature, the preferred core unit is regarded as a multivalent substituent of multiple parent structures, the dendrons, and is named according to the rules of organic chemistry multiplicative nomenclature [14].

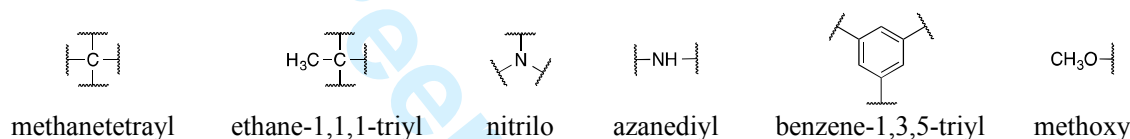
DH-2.7.2 Concatenation is the method used for formation of multipart multivalent core unit names. The central multiplicative component is cited first, followed by a multiplicative prefix such as di-, tri-, etc., or bis-, tris- etc., and then, in order and in the dendron direction, the names of the successive di- or polyvalent substituent components. Only one multiplicative prefix is allowed in the name, e.g. ethane-1,1,1-triyltris(4,1-phenyleneoxy), not ethane-1,1,1-triyltris(4,1-phenylene)tris(oxy).

DH-2.7.3 Numbering of the components of a core unit, when necessary, is achieved by attributing the lowest locants to the atoms that are at the end of the component, i.e. nearest to the dendron(s), except when the component has a fixed numbering. The locants for the points of attachment of the dendrons are cited last. When there is a choice, locants are cited in increasing numerical order.

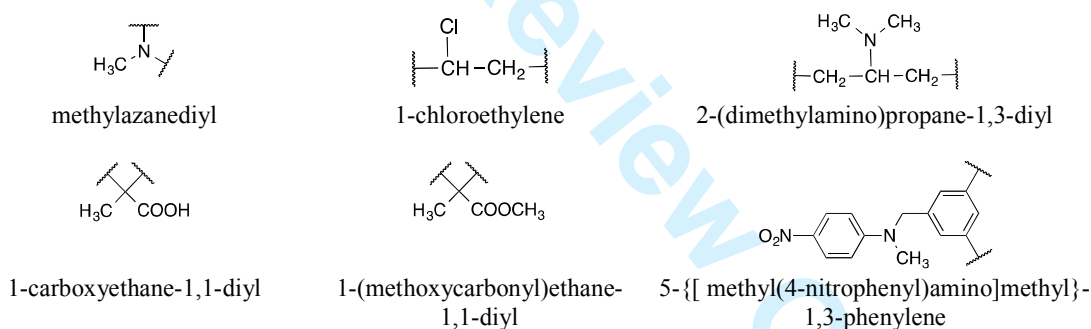
DH-2.7.4 Names that are preferred in polymer structure-based nomenclature should be used, e.g. ethylene instead of ethane-1,2-diyl.

DH-2.7.5 Examples of core unit names in dendrimer multiplicative nomenclature:

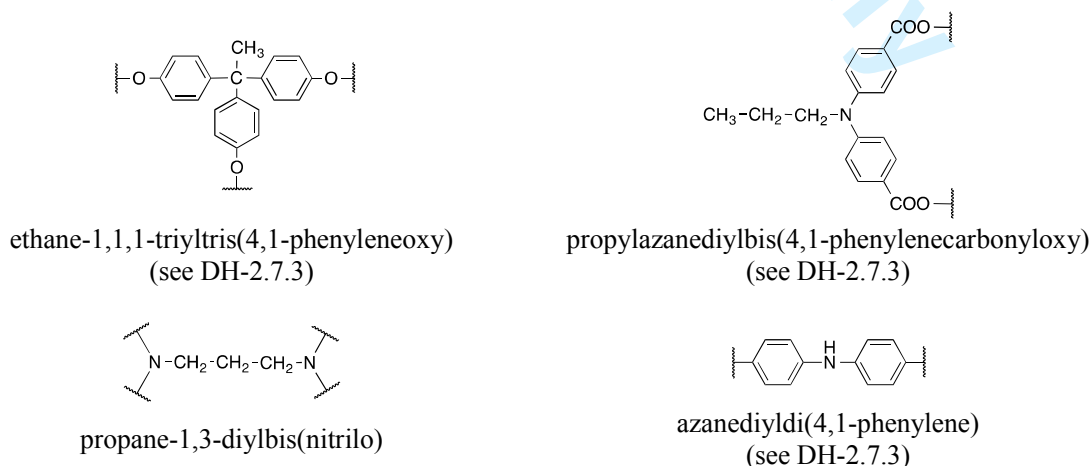
a) Monovalent and multivalent simple core units:

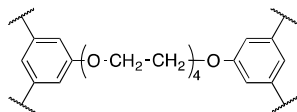


b) Multivalent substituted simple core units:

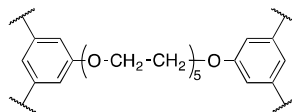


c) Symmetrical complex core units:



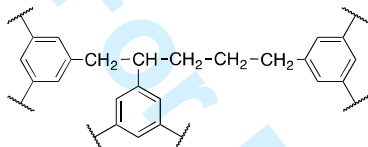


oxybis[ethyleneoxyethyleneoxybenzene-5,1,3-triyl]
(see DH-2.7.3)

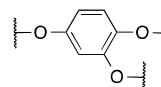


ethylenebis[oxyethyleneoxyethyleneoxybenzene-5,1,3-triyl]
(see DH-2.7.3)

d) Unsymmetrical complex core units



pentane-1,2,5-triyltri(benzene-5,1,3-triyl)



benzene-1,2,4-triyltris(oxy)

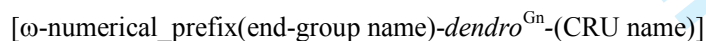
DH-2.8 Naming the preferred core unit of a dendrimer molecule in substitutive nomenclature

In substitutive nomenclature, the parent hydride of simple core units or the parent hydride of the central multiplicative component of multipart core units are chosen as parent structures and named according to organic chemistry nomenclature rules [14].

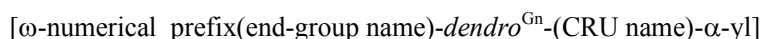
Note: Names preferred in polymer structure-based nomenclature should be used, e.g. ethylene instead of ethane-1,2-diyl.

DH-2.9 Naming a regular dendron

DH-2.9.1 In multiplicative nomenclature, a regular dendron is named by citing the name of the end-groups preceded by ω - followed by the italicized prefix *-dendro*^{G_n}-, where n is the number of generations of the dendron, and the parenthesized name of the preferred constitutional repeating unit. The number of end-groups is indicated by a numerical prefix (di-, tri-, etc. or bis, tris, tetrakis, etc.) before the name of the end-groups. Dendron name is enclosed in parentheses, brackets or braces, as appropriate:



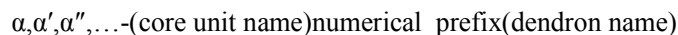
DH-2.9.2 In substitutive nomenclature, dendron name is followed by $-\alpha$ -yl, indicating that its senior end (the free valence) is connected to the parent structure (core unit or polymer chain). The CRU name is the same as that defined in multiplicative nomenclature.



DH-2.10 Naming regular dendrimers with a symmetrical core unit

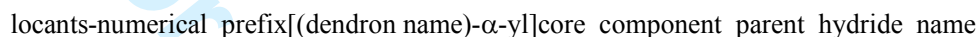
DH-2.10.1 Multiplicative nomenclature

In multiplicative nomenclature, a regular dendrimer is named by citing in order the name of the core unit preceded by $\alpha, \alpha', \alpha'', \dots$ -, depending on the number of dendrons, a numerical prefix (bis, tris, etc.) indicating the number of dendrons, followed by the name of the dendron(s).



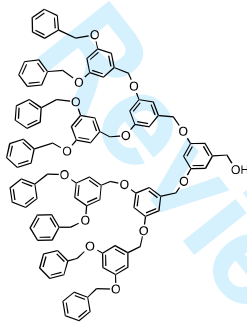
DH-2.10.2 Substitutive nomenclature

In substitutive nomenclature, a dendrimer is named as the dendron-substituted parent hydride of the innermost core component (DH-2.8), according to organic nomenclature rules [14]. Dendrons and substituents are cited in alphabetical order, without taking into account numerical prefixes.

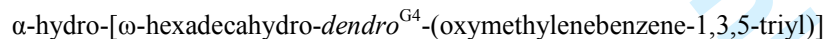


Note: Dendron name is the same in multiplicative and in substitutive nomenclature. In substitutive nomenclature dendron name is followed by the $-\alpha\text{-yl}$ suffix (see DH-2.9.2).

Example 1. Poly(benzyl ether)-type dendrimer with one regular dendron and a monovalent simple core unit [24].



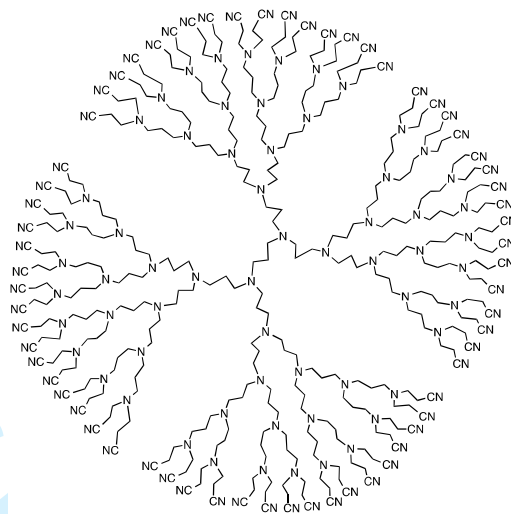
The preferred CRU is oxymethylenebenzene-1,3,5-triyl (branch points last and locants cited in the dendron direction). The preferred core unit is a single hydrogen atom and the benzyloxy end-groups must be considered as composed of one CRU and two hydro end-groups, since this leads to a higher number of generations ($G = 4$). Multiplicative nomenclature is preferred:



In order to name this dendrimer by substitutive nomenclature, one CRU should be included in the core unit since substitution to hydrogen is not possible. Consequently, the dendrimer should be regarded as formed of two 3-generation dendrons and a substituted simple core unit, 5-hydroxymethylbenzene.



Example 2. Regular 4-dendron poly(propylene imine)-type dendrimer [25].



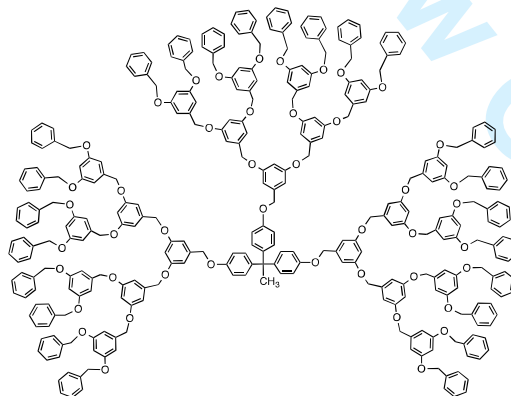
The preferred CRU is propane-1,3-diyl nitrilo (branch point last), leading to 2-cyanoethyl end-groups and to a propane-1,3-diylbis(nitrilo) symmetrical core unit. $G = 4$ for each dendron. Dendrimer multiplicative nomenclature is preferred:

$\alpha, \alpha', \alpha'', \alpha'''$ -[propane-1,3-diylbis(nitrilo)]tetrakis[ω -hexadecakis (2-cyanoethyl)-*dendro*^{G⁴}-(propane-1,3-diyl nitrilo)]

Dendrimer substitutive nomenclature name:

N^1, N^1, N^2, N^2 -[ω -hexadecakis(2-cyanoethyl)-*dendro*^{G⁴}-(propane-1,3-diyl nitrilo)- α -yl]propane-1,3-diamine

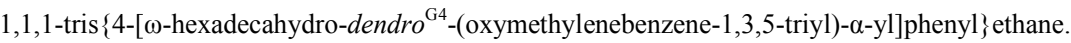
Example 3. Regular 3-dendron poly(benzyl ether)-type dendrimer [15].



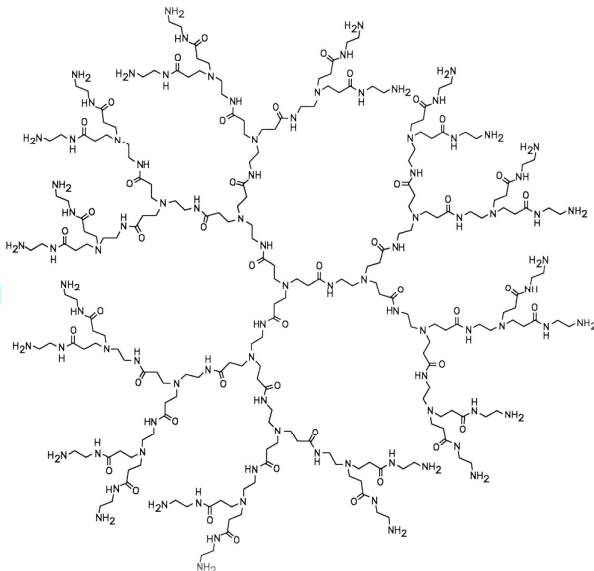
The preferred CRU is oxymethylenebenzene-1,3,5-triyl (branch point last), leading to the ethane-1,1,1-triyltri(4,1-phenylene) core unit. The benzyloxy end-groups must be considered as composed of an oxymethylenebenzene-1,3,5-triyl CRU and 2 hydro end-groups, since this leads to a higher number of generations for each dendron ($G = 4$). Dendrimer multiplicative nomenclature is preferred:

$\alpha, \alpha', \alpha''$ -[ethane-1,1,1-triyltri(4,1-phenylene)]tris[ω -hexadecahydro-*dendro*^{G⁴}-(oxymethylenebenzene-1,3,5-triyl)]

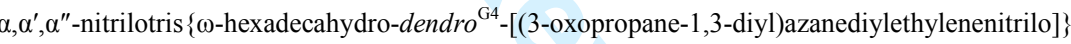
Dendrimer substitutive nomenclature name:



Example 4. Regular 3-dendron poly(amidoamine)-type dendrimer (PAMAM) [3].



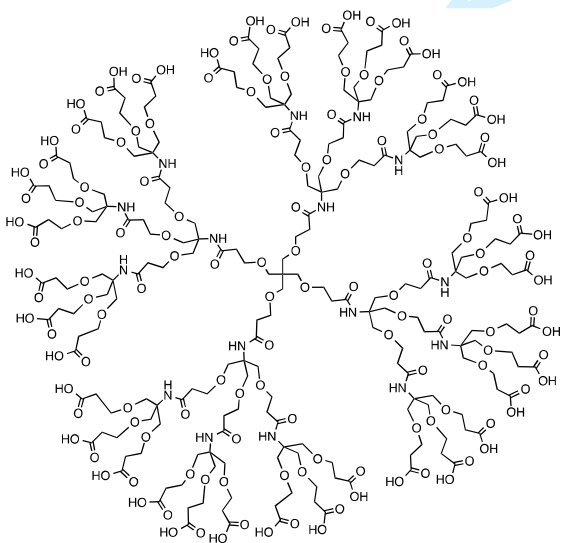
The preferred CRU is (3-oxopropane-1,3-diyl)azanediylethylenenitrilo, leading to hydro end-groups and nitrilo core (*G* = 4). Dendrimer multiplicative nomenclature is preferred:



Dendrimer substitutive nomenclature can also be applied:



Example 5. Regular 4-dendron poly(ether amido)-type dendrimer [26].



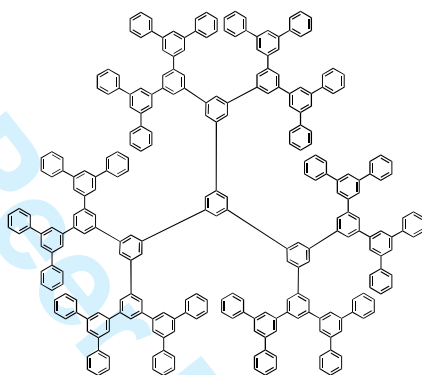
The preferred CRU is methyleneoxy(3-oxopropane-1,3-diyl)azanediylmethanetetrayl (branch points last). This leads to a methanetetrayl symmetrical core unit and to (2-carboxyethoxy)methyl end-groups (*G* = 2). Dendrimer multiplicative nomenclature is preferred:

$\alpha, \alpha', \alpha'', \alpha'''$ -(methanetetrayl)tetrakis{ ω -nonakis[(2-carboxyethoxy)methyl]-*dendro*^{G²}-[methyleneoxy(3-oxopropane-1,3-diyl)azanediylmethanetetrayl]}

Dendrimer substitutive nomenclature name:

tetrakis{ ω -nonakis[(2-carboxyethoxy)methyl]-*dendro*^{G²}-[methyleneoxy(3-oxopropane-1,3-diyl)azanediylmethanetetrayl] α -yl}methane

Example 6. Regular 3-dendron dendrimer in which the core unit and CRUs have the same structure [27].



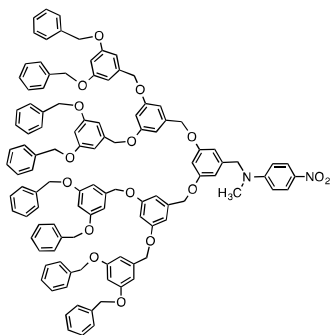
The preferred CRU is benzene-1,3,5-triyl, leading to a benzene-1,3,5-triyl core unit and hydro end-groups ($G = 4$). Dendrimer multiplicative nomenclature is preferred:

$\alpha, \alpha', \alpha''$ -benzene-1,3,5-triyltris[ω -hexadecahydro-*dendro*^{G⁴}-(benzene-1,3,5-triyl)]

Dendrimer substitutive nomenclature name:

1,3,5-tris[ω -hexadecahydro-*dendro*^{G⁴}-(benzene-1,3,5-triyl)- α -yl]benzene

Example 7. Regular 2-dendron poly(benzyl ether)-type dendrimer [28].



This dendrimer is similar to that discussed in Example 1. However, the core unit is now a substituted divalent simple core unit (1,3-phenylene) and the dendrimer must be regarded as a 3-generation regular one with two dendrons. Dendrimer multiplicative nomenclature is preferred:

$\alpha, \alpha'-(5-\{[methyl(4-nitrophenyl)amino]methyl\}-1,3-phenylene)bis[\omega-octahydro-*dendro*^{G³}-(oxymethylenebenzene-1,3,5-triyl)]$.

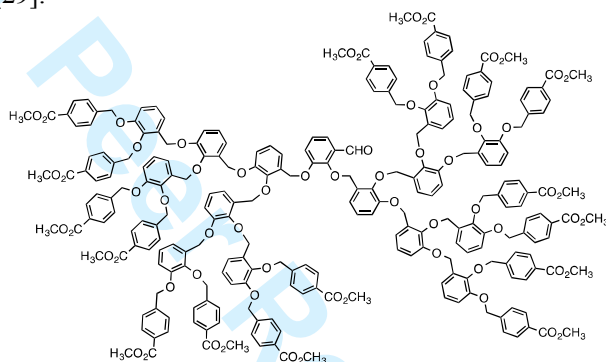
The dendrons are attached to atoms 1 and 3 of the core unit (lowest locants). Numerical order 1,3 is preferred to 3,1. This case is different from the 4,1-phenylene component of DH-2.7.5.c where the phenylene unit bears only one dendron. The corresponding locant is numbered 1 (closest to the dendron), hence the 4,1 orientation.

Dendrimer substitutive nomenclature name:

1,3-bis[ω -octahydro-*dendro*^{G3}-(oxymethylenebenzene-1,3,5-triyl)- α -yl]-5-[[methyl(4-nitrophenyl)amino]methyl]benzene.

Substituent ω -octahydro-*dendro*... is cited first since "hydro" alphabetizes earlier than "methyl" (DH-2.10.2)

Example 8. Regular poly(benzyl ether)-type dendrimer with a substituted divalent symmetrical core unit and two dendrons [29].



The preferred CRU is oxymethylenebenzene-1,2,3-triyl, leading to [4-(methoxycarbonyl)phenyl]methoxy end-groups and to a formyl-substituted 1,2-phenylene divalent simple core unit ($G = 3$). Dendrimer multiplicative nomenclature is preferred:

α, α' -(3-formyl-1,2-phenylene)bis(ω -octakis[[4-(methoxycarbonyl)phenyl]methoxy]-*dendro*^{G3}-[oxymethylenebenzene-1,2,3-triyl]).

Dendrimer substitutive nomenclature name:

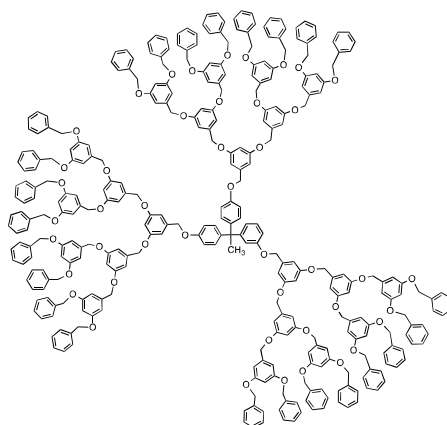
3-formyl-1,2-bis(ω -octakis[[4-(methoxycarbonyl)phenyl]methoxy]-*dendro*^{G3}-[oxymethylenebenzene-1,2,3-triyl]- α -yl)benzene.

DH-2.11 Naming regular dendrimers with an unsymmetrical core unit

DH-2.11.1 Regular dendrimers with unsymmetrical core units are named by dendrimer substitutive nomenclature, as the dendron-substituted parent hydride of the innermost core component (DH-2.8, DH-2.10.2).

DH-2.11.2 Identical dendrons are cited in increasing numerical order of locants.

Example 9. Regular poly(benzyl ether)-type dendrimer with an unsymmetrical multipart core unit.

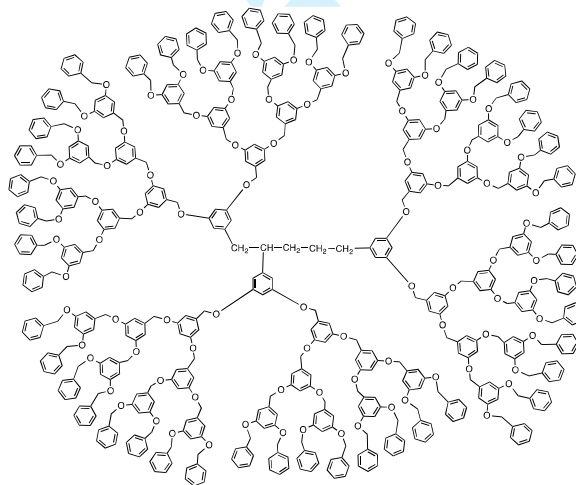


This regular 3-dendron dendrimer presents an unsymmetrical multipart core unit. Substitutive nomenclature must be used:

1-{3-[ω-hexadecahydro-*dendro*^{G4}-(oxymethylenebenzene-1,3,5-triyl)-α-yl]phenyl}-1,1-bis{4-[ω-hexadecahydro-*dendro*^{G4}-(oxymethylenebenzene-1,3,5-triyl)-α-yl]phenyl}ethane.

The "1-{3-" dendron is cited before the two "1-{4-" dendrons, according to DH-2.11.2.

Example 10. Regular 6-dendron poly(benzyl ether)-type dendrimer with an unsymmetrical multipart core unit.



This regular 6-dendron dendrimer presents an unsymmetrical core unit. Substitutive nomenclature must be used:

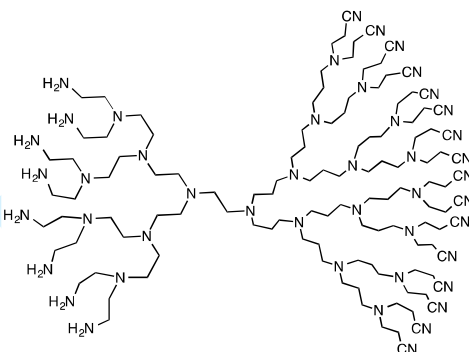
1,2,5-tris{3,5-bis[ω-hexadecahydro-*dendro*^{G4}-(oxymethylenebenzene-1,3,5-triyl)-α-yl]phenyl}pentane

DH-2.12 Naming irregular dendrimers with a symmetrical core unit

DH-2.12.1 Irregular dendrimers are named by dendrimer substitutive nomenclature, as the dendron-substituted parent hydride of the innermost core component (DH-2.8, DH-2.10.2).

DH-2.12.2 Dendrons and substituents are cited in alphabetical order, without taking into account numerical prefixes. If dendrons differ only by the number of generations, the smallest is cited first.

Example 11. Irregular dendrimer with a symmetrical core unit.

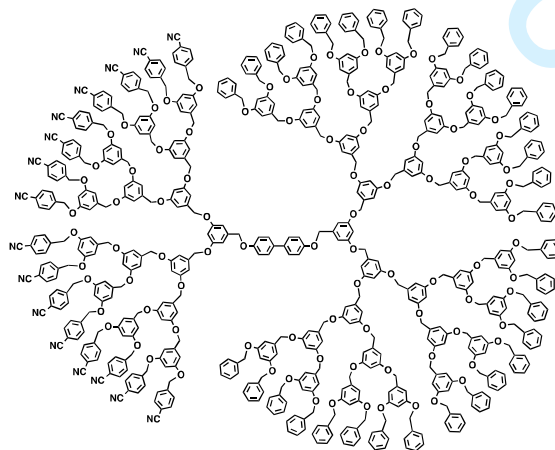


This irregular dendrimer is composed of two parts: on the left side, a hydro-terminated dendron with ethylenitrilo CRUs (branch points last in the dendron direction) and a nitrilo simple core unit ($G = 4$). On the right side, two identical dendrons are attached to the nitrilo core. They are formed of propane-1,3-diynitrilo CRUs (branch points last in the dendron direction) and of 2-cyanoethyl end-groups ($G = 3$). Dendrimer substitutive nomenclature must be used:

bis{ ω -octakis(2-cyanoethyl)-*dendro*^{G³}-(propane-1,3-diynitrilo)- α -yl}[ω -hexadecahydro-*dendro*^{G⁴}-(ethylenitrilo)- α -yl]azane

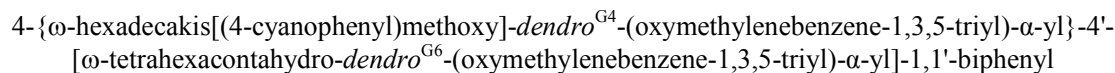
Since cyano alphabetizes earlier than hydro, the 2-cyanoethyl-terminated dendron is cited first (DH-2.12.2).

Example 12. Irregular poly(benzyl ether)-type dendrimer with a symmetrical core unit [30].



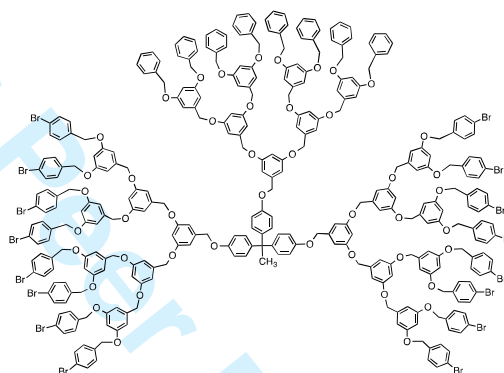
This irregular dendrimer is composed of two parts: the left part consists of a 4-cyanobenzyloxy-terminated dendron with an oxymethylenebenzene-1,3,5-triyl CRU (branch point last) and $G = 4$. The right one consists of a hydro-terminated dendron with the same oxymethylenebenzene-1,3,5-triyl CRU

and $G = 6$. The core unit is a biphenyl moiety, where, according to organic chemistry nomenclature rules, the two phenyl-connecting carbons must be numbered 1,1' (fixed numbering). Dendrimer substitutive nomenclature must be used:

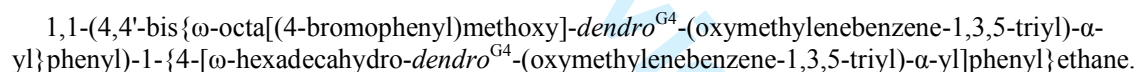


Since cyano alphabetizes earlier than hydro, the (4-cyanophenyl)methoxy -terminated dendron is cited first (DH-2.12.2).

Example 13. Irregular poly(benzyl ether)-type dendrimer [24].



This irregular dendrimer is composed of two 4-bromobenzyloxy-terminated dendrons ($G = 3$), one hydro-terminated dendron ($G = 4$) (see Example 3). Dendrimer substitutive nomenclature must be used:

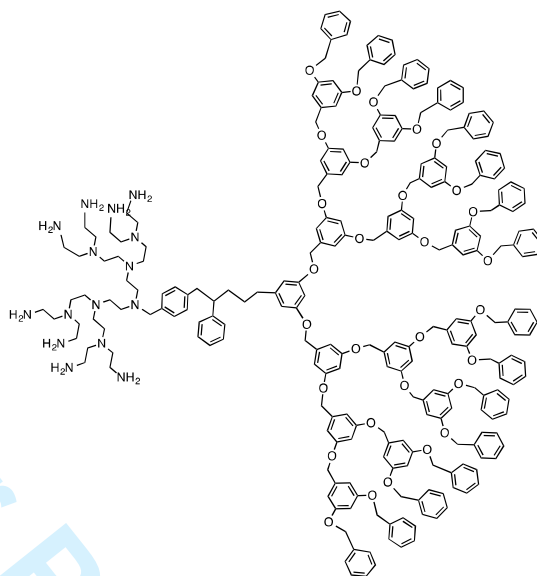


Bromo-terminated dendrons are cited first, since bromo alphabetizes earlier than hydro (DH-2.12.2).

DH-2.13 Naming irregular dendrimers with an unsymmetrical core unit

An irregular dendrimer with an unsymmetrical core unit is named by substitutive nomenclature as being the dendron-substituted parent hydride of the innermost core component, according to organic nomenclature rules [14].

Example 14. Irregular dendrimer with an unsymmetrical core unit.



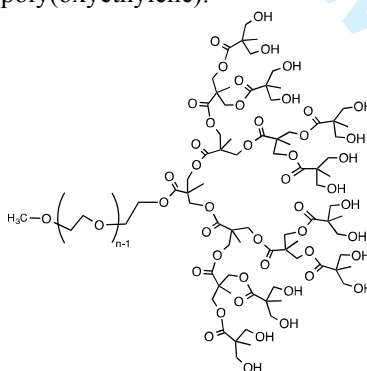
This irregular dendrimer is based on the unsymmetrical core unit of Example 11. Dendrimer substitutive nomenclature must be used. The 1,2,5 (lowest possible) locant set is chosen for the pentanetriyl innermost component. Dendron and phenyl substituents are cited in alphabetical order (DH-2.11.3.).

1-[4-(bis[ω-octahydro-dendro]^{G3}-(ethylenenitrilo)-α-yl)amino)methyl]phenyl]-5-{3,5-bis[ω-hexadecahydro-dendro]^{G4}-(oxymethylenebenzene-1,3,5-triyl)-α-yl]phenyl}-2-phenylpentane

DH-2.14 Naming dendritic block polymers

Dendritic block-copolymers are named as dendron-substituted polymers, according to polymer nomenclature rules. The multiplicative nomenclature may, however, be used in the specific case of uniform polymers of exactly known chain length.

Example 15. Dendron-substituted poly(oxyethylene).



Depending on the position of poly(oxyethylene) parentheses, this dendritic block copolymer can be regarded as either:

- A poly(oxyethylene) with a dendron-substituted methyl end-group at one end and a methoxy end-group at the other,
- A poly(oxyethylene) with a dendron-substituted methoxy end-group at one end and a methyl end-group at the other.

The α -end (i.e. the senior end) of a polyoxyethylene chain is connected to the senior component of its last CRU, i.e. oxy. Therefore, the α -end can only be a methyl or a substituted methyl group and is cited first, leading to:

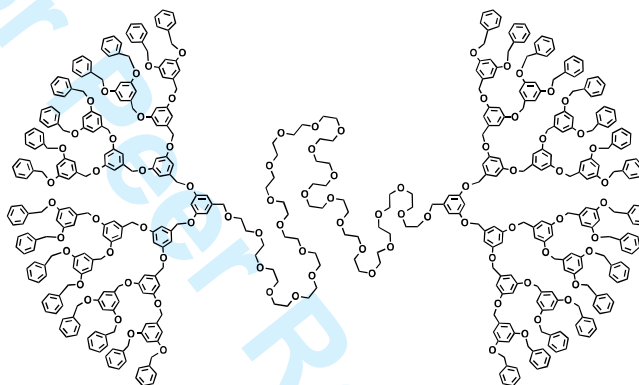
α -({ ω -hexadecakis(hydroxymethyl)-*dendro*^{G4}-[methyleneoxy(1-oxo-2-methylethane-1,2,2-triyl)]- α -yl}methyl)- ω -methoxypoly(oxyethylene) (preferred)

or:

α -methyl- ω -({ ω -hexadecakis(hydroxymethyl)-*dendro*^{G4}-[methyleneoxy(1-oxo-2-methylethane-1,2,2-triyl)]- α -yl}methoxy)poly(oxyethylene)

Since hydroxymethyl alphabetizes earlier than methyl, the first name is preferred.

Example 16. Dendron-substituted poly(oxyethylene) [31].



In this example, the chain linking the two 5-generation dendrons is formed of exactly one ethylene unit and 23 oxyethylene units and can be named oxybis[undeca(ethyleneoxy)ethylene] according to multiplicative nomenclature rules. The molecule can be regarded as a dendrimer molecule and named according to dendrimer multiplicative nomenclature rules:

α, α' -{oxybis[undeca(ethyleneoxy)ethylene]}; bis[ω -dotriacontahydro-*dendro*^{G5}-(oxymethylenebenzene-1,3,5-triyl)]

The substitutive name is derived from polymer nomenclature, with dendrons as end-groups. The dendron-substituted ethyl group is substituent to the α -end (oxy) of the oxyethylene chain:

α -{2-[ω -dotriacontahydro-*dendro*^{G5}-(oxymethylenebenzene-1,3,5-triyl)- α -yl]ethyl}- ω -[ω -dotriacontahydro-*dendro*^{G5}-(oxymethylenebenzene-1,3,5-triyl)- α -yl]tricosapoly(oxyethylene).

If the central poly(oxyethylene) chain were non-uniform, the multiplicative nomenclature could no longer be applied. The substitutive name of the dendritic block-copolymer would be:

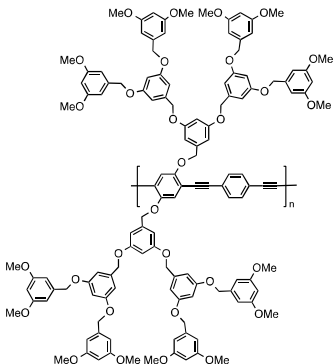
α -{2-[ω -dotriacontahydro-*dendro*^{G5}-(oxymethylenebenzene-1,3,5-triyl)- α -yl]ethyl}- ω -[ω -dotriacontahydro-*dendro*^{G5}-(oxymethylenebenzene-1,3,5-triyl)- α -yl]poly(oxyethylene)

DH-2.15 Naming dendritic graft polymers

In a dendritic graft polymer, the chain is considered to be composed of dendron-substituted constitutional repeating units and named according to the rules established for regular or irregular single strand copolymers [12]:

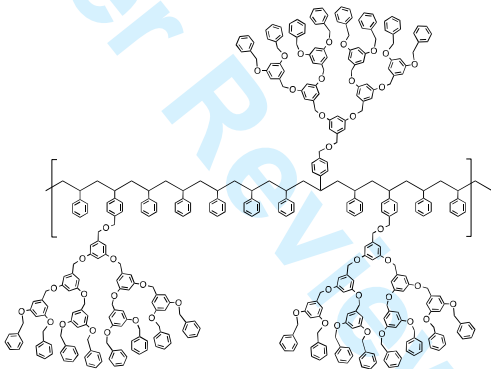
poly(CRU1) ; poly(CRU1/CRU2) ; poly(CRU1/CRU2/CRU3) ; etc.,
where one or more types of CRUs are dendron-substituted.

Example 17. Dendritic graft poly[(1,4-phenylene)ethyne-1,2-diyl] [32].



poly({2,5-bis[ω-octamethoxy-*dendro*^{G3}-(oxymethylenebenzene-1,3,5-triyl)-α-yl]-1,4-phenylene}ethyne-1,2-diyl(1,4-phenylene)ethyne-1,2-diyl)

Example 18. Dendritic graft polystyrene copolymer [31].



poly[1-(4-{[ω-hexadecahydro-*dendro*^{G4}-oxymethylene(benzene-1,3,5-triyl)-α-yl]methyl}phenyl)ethylene/1-phenylethylene]

DH-3 NOMENCLATURE FOR HYPERBRANCHED POLYMERS AND OLIGOMERS

Multiplicative nomenclature is not allowed for hyperbranched polymers. They are named according to conventional structure-based polymer nomenclature [12]. Polymer CRUs, end-groups and core unit are chosen and named as the corresponding dendrimer moieties. The core unit and end-groups are regarded as the α - and ω -ends of polymer chains, respectively.

This nomenclature is applicable to hyperbranched polymers where a dendron direction and a core unit can be defined, e.g. for hyperbranched polymers obtained by reacting AB_x -type monomers or by reacting AB_x -type monomers with B_y -type monomers, where A and B represent mutually reactive groups.

In all other cases, ill-defined polymer structures are obtained, to which structure-based name can hardly be given. In this case, source-based nomenclature [12] is preferred.

DH-3.1 Choice and name of the preferred constitutional repeating unit

The preferred constitutional repeating unit is chosen and named according to the rules defined for dendrimers (DH-2.2 and DH-2.5)

DH-3.2 Choice and name of the preferred core unit

The preferred core-unit is chosen according to the rules defined for dendrimers (DH-2.4). It is named substitutively, according to organic chemistry nomenclature rules [14], and is regarded as the α -end of the polymer chain.

Note: See also DH-2.7.

DH-3.3 Naming the end-groups

The preferred end-groups are chosen according to the rules defined for dendrimers (DH-2.3). They are named substitutively, according to organic chemistry nomenclature rules [14], and are considered to be ω -ends of the polymer chain.

Note: The number of end-groups cannot be specified in hyperbranched polymer names.

DH-3.4 Naming hyperbranched polymers and oligomers

A hyperbranched oligomer or polymer is named by citing in order the name of the core unit preceded by α -, the name(s) of the end-groups(s) preceded by ω - and, after the italicized prefix *-hyper-* and prefix *poly*, the parenthesized name(s) of the preferred constitutional repeating unit(s) of lower connectivity followed by the preferred constitutional repeating unit(s) of higher connectivity, if any. All terms are separated by hyphens.

Note 1: The prefix *-hyper-* preceding the prefix 'poly' indicates the hyperbranched nature of the polymer, i.e. the presence of an unspecified number of linear or semi-dendritic CRUs in the polymer chain.

Note 2: When the polymer contains more than one type of CRU and/or blocks or grafts, the rules of polymer nomenclature [12] should be followed.

Note 3: When the CRU contains more than one type of component of connectivity larger than 2, the component of highest connectivity should be cited last. If a further choice is needed, the component of highest seniority should be cited last.

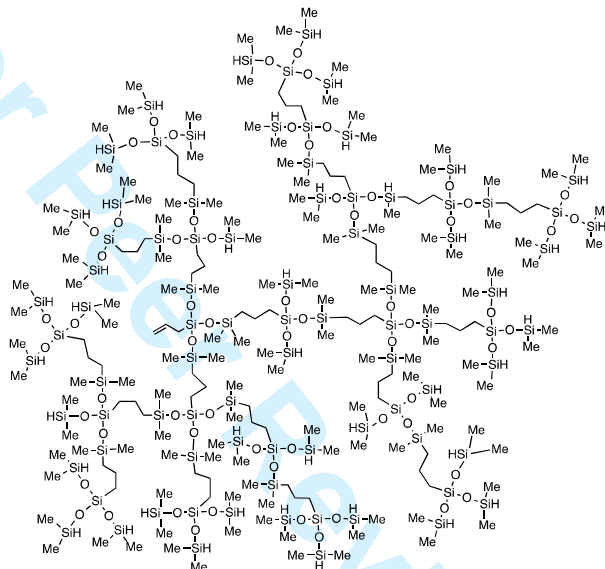
Note 4: Whether the compound is to be considered oligomeric or polymeric can be specified by the prefix 'oligo' or 'poly' preceding the parenthesized name of the preferred CRU.

Generic formats of the names are:

α -(core unit name)- ω -(end-group1 name)- ω -(end-group2 name)-...-*hyper*-poly(CRU)

α -(core unit name)- ω -(end-group1 name)- ω -(end-group2 name)-...-*hyper*-oligo(CRU)

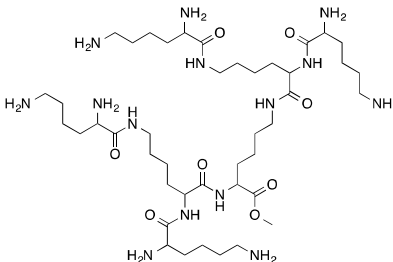
Example 19. Hyperbranched polymer with dimethylsiloxo end-groups and a (prop-2-en-1-yl)silanetriyl core [33].



α -(prop-2-en-1-ylsilanetriyl)- ω -(dimethylsiloxo)-*hyper*-poly[oxy(dimethylsilanediyl)propane-1,3-diylsilanetetrayl].

Source-based name: poly{3-[(dimethylsilyl)oxy]-1,1,5,5-tetramethyl-3-(prop-2-en-1-yl)trisiloxane}

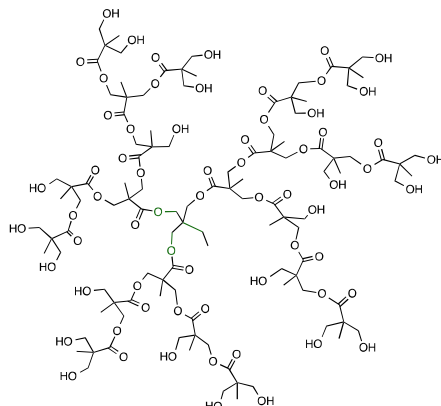
Example 20. Hyperbranched poly(L-lysine) with amino end-groups and a methoxycarbonyl-substituted hexane core unit [34].



The CRU is azanediyl(1-oxohexane-1,2,6-triyl). Locants 1,2,6 are cited in the dendron direction.

α -[1-(methoxycarbonyl)pentane-1,5-diyl]- ω -amino-*hyper*-poly[azanediyl(1-oxohexane-1,2,6-triyl)]

Source-based name: poly(L-lysine).

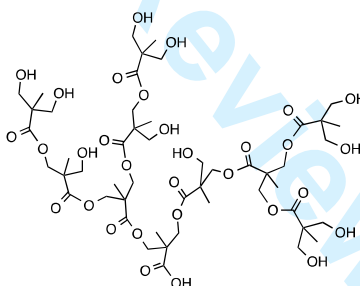
Example 21 [8]

α -(propane-1,1,1-triyl)- ω -(hydroxymethyl)-*hyper*-poly[methyleneoxy(2-methyl-1-oxoethane-1,2,2-triyl)]

Source-based name:

α -(propane-1,1,1-triyl)- ω -(hydroxymethyl)poly[3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic acid].

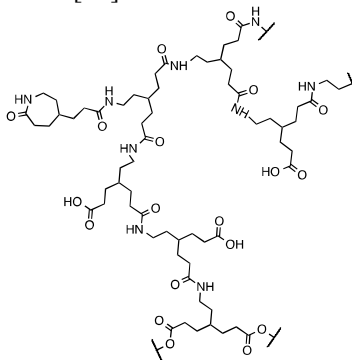
Note: This polymer is synthesized from 3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic acid] and (propane-1,1,1-triyl)trimethanol. The source-based name should specify the nature of the core unit (' α -' end-group) and of the end groups (' ω -' end groups).

Example 22 [8].

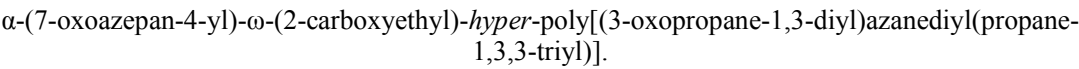
α -(1-carboxyethane-1,1-diyl)- ω -(hydroxymethyl)-*hyper*-poly[methyleneoxy(2-methyl-1-oxoethane-1,2,2-triyl)]

Source-based name: poly[3-hydroxy-2-(hydroxymethyl)-2-methylpropanoic acid]

Example 23. Hyperbranched polymer prepared by the ring-opening self-polymerization of a carboxyethyl-functionalized caprolactam [35].

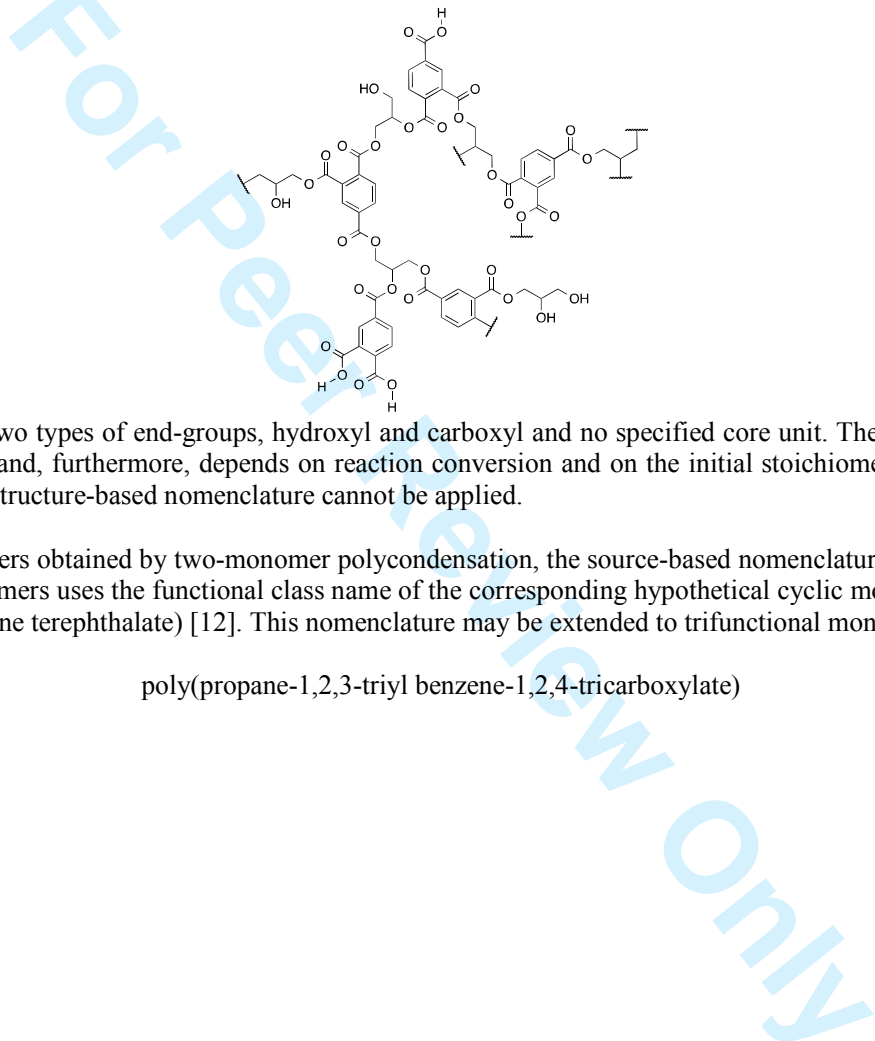


The preferred CRU is (3-oxopropane-1,3-diyl)azanediyl(propane-1,3,3-triyl) (branch points last). In the CRU name, locants are numbered and cited in the dendron direction.



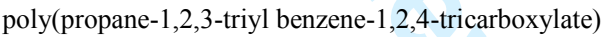
Source-based polymer name: poly[3-(7-oxoazepan-4-yl)propanoic acid].

Example 24. Hyperbranched polyester prepared from propane-1,2,3-triol and benzene-1,2,4-tricarboxylic acid.



There are two types of end-groups, hydroxyl and carboxyl and no specified core unit. The structure is ill-defined and, furthermore, depends on reaction conversion and on the initial stoichiometric ratio of reactants. Structure-based nomenclature cannot be applied.

For polyesters obtained by two-monomer polycondensation, the source-based nomenclature for single-strand polymers uses the functional class name of the corresponding hypothetical cyclic monomer, e.g. poly(ethylene terephthalate) [12]. This nomenclature may be extended to trifunctional monomers:



List of abbreviations and symbols

CU	Constitutional unit	(DH-1.6)
CRU	Constitutional repeating unit	(DH-1.7)
<i>c</i>	Connectivity (of a constitutional unit)	(DH-1.5)
<i>D</i> _{br}	Degree of branching	(DH-1.9)
<i>G</i>	number of generations	(DH-1.32)

List of definitions

DH-1.1	branch
DH-1.2	branch constitutional repeating unit
DH-1.3	branch point
DH-1.4	chain
DH-1.5	connectivity (of a constitutional unit)
DH-1.6	constitutional unit (CU)
DH-1.7	constitutional repeating unit (CRU)
DH-1.8	core unit
DH-1.9	degree of branching
DH-1.10	dendrimer
DH-1.11	dendrimer molecule
DH-1.12	dendritic block macromolecule
DH-1.13	dendritic constitutional repeating unit
DH-1.14	dendritic graft macromolecule
DH-1.15	dendritic macromolecule
DH-1.16	dendritic polymer
DH-1.17	dendron
DH-1.18	dendron direction
DH-1.19	end-group
DH-1.20	focal unit
DH-1.21	generation (in a dendron)
DH-1.22	hyperbranched macromolecule
DH-1.23	hyperbranched oligomer
DH-1.24	hyperbranched oligomer molecule
DH-1.25	hyperbranched polymer
DH-1.26	irregular dendrimer
DH-1.27	irregular macromolecule
DH-1.28	irregular dendrimer molecule
DH-1.29	irregular dendron
DH-1.30	linear constitutional repeating unit
DH-1.31	macromolecule, polymer molecule
DH-1.32	number of generations (of a dendron)
DH-1.33	number of generations (of a regular dendrimer molecule)
DH-1.34	number of pseudo-generations (of a hyperbranched polymer)
DH-1.35	oligomer
DH-1.36	oligomer molecule
DH-1.37	polymer
DH-1.38	regular dendrimer
DH-1.39	regular dendrimer molecule
DH-1.40	regular dendron
DH-1.41	regular macromolecule
DH-1.42	semi-dendritic constitutional repeating unit
DH-1.43	terminal constitutional repeating unit

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