Dendritic and Star Polymers: Classification, Nomenclature, Structure Representation, and Registration in the DuPont SCION Database

John L. Schultz† and Edward S. Wilks*

E. I. du Pont de Nemours and Company, Wilmington, Delaware 19880

Received October 10, 1997

Classification, nomenclature, and structure representation are presented for dendritic and star polymers in SCION, a DuPont proprietary scientific and technical online database. The problems of registering dendritic and hyperbranched structural repeating units (SRUs) with odd numbers of crossing bonds are described, and solutions to circumvent registration system limitations are discussed. A systematic approach to the classification, nomenclature, and structure representation in SCION of 20 categories of star polymers is described.

1. INTRODUCTION

SCION is a DuPont proprietary online database that uses the Chemical Abstracts Service (CAS) Registry System (CASRS) for polymer registration and Messenger software for searching.[1] The file comprises a bibliographic file and a chemical structure file. The two files work in a manner that parallels the functions and interactions of File CA and File Registry published by the CAS of the American Chemical Society (ACS). The chemical file of the SCION database, described earlier,[1] follows CAS structure conventions except in the polymer field, where appreciable differences exist. Among these major differences are conventions for dendritic, star, star-block, and star-branched polymers, and these are described in this paper.

Registration of polymers is executed manually for DuPont by CAS keyboarding personnel. This paper discusses classification, nomenclature, structure representation, and registration rules to accompany manual encoding of polymers, but the principles might be used for an automated polymer registration system.

2. BACKGROUND

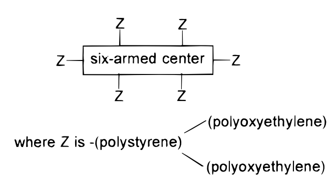
Dendritic, star, star-block, and star-branched polymers are discussed together because there is overlapping technology that makes it difficult to discuss them separately. In the last decade there has been a sharp rise in the interest of these types of polymers; for example, at the 210th ACS meeting (August, 1995), out of a total of 302 presentations in the Division of Polymeric Materials: Science and Engineering (PMSE), 44 (15%) of the contributions (32 papers and 12 posters) were on dendritic, hyperbranched, and star polymers, and combinations of these. At the 214th ACS meeting (September, 1997), >100 papers on dendritic and hyperbranched polymers were presented.

According to Tomalia *et al.*,[2a] dendritic polymers, also called dendrimers,[2a] have three distinguishing architectural features: an initiator core, interior layers (generations) composed of repeating units radially attached to the initiator core, and an exterior or surface of terminal functionality attached to the outermost generation. Dendrimers differ from classical polymers or oligomers by their extraordinary symmetry, high branching, and maximized (telechelic) terminal functionality. Dendrimer synthesis is accomplished by a variety of strategies involving time-sequenced propagation techniques. The resulting dendrimers grow in a geometrically progressive fashion. Chemical bridging of these dendrimers leads to "Starburst" polymers[2b] ("Starburst" is a registered trademark of the Dow Chemical Company).

De Brabander *et al.*[3] define a dendrimer as a highly branched (degree of branching = 1), highly functionalized macromolecule with a well-defined structure. Newkome[4] has described a systematic nomenclature for cascade (i.e., dendritic) polymers.

However, the term dendrimer is interpreted by other scientists as having a much broader meaning than the ones described by Tomalia, de Brabander, and Newkome. For example, Cloutet *et al.*[5] describe the polymer shown as example 2.1 as a "dendritic block" polymer, although it might be more appropriate to call it a branched star-block polymer.

Example 2.1. Dendritic block polymer (according to Cloutet *et al.*).

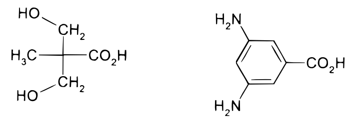


According to Turner,[6] hyperbranched polymers are highly branched, non-cross-linked polymers prepared by the step-growth polymerization of A_xB (or AB_x) monomers, where x is an integer. Thus, A_2B means that for every two type A reactive groups there is one type B reactive group, whereas AB_2 means that for every one type A reactive group there are two type B reactive groups. AB_2 and AB_3 (or A_2B and A_3B) are the most commonly encountered polymers because more highly branched types such as AB_4 (or A_4B) types tend to be so sterically crowded that polymerization is difficult unless the reactive groups are well separated.

Typical AB_2 (or A_2B) monomers are shown as examples 2.2 (left structure below) and 2.3 (right structure below).

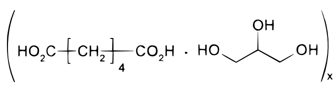
† Retired.

S0095-2338(97)00090-5 CCC: $15.00
Published on Web 02/19/1998



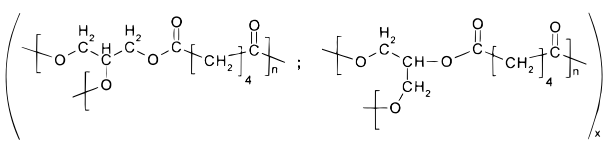
However, it is not necessary that ***every*** monomer unit in a hyperbranched polymer have a connectivity greater than two. Connectivity is the number of crossing bonds emanating from a monomer unit. A crossing bond in an SRU is a bond that crosses one of the limiting parentheses or brackets. Example 2.4.1 shows one in which every other monomer unit has a connectivity of three. The possibility of hypercrosslinking (i.e., formation of macrocycles) is present but can be minimized by use of appropriate synthetic techniques, such as polymerization at high dilution.

Example 2.4.1. Polyester from adipic acid and glycerol-source-based representation.



The structure-based representation of this polymer (example 2.4.2) necessitates at least two structural repeating units (SRUs), both with three crossing bonds.

Example 2.4.2. Polyester from adipic acid and glycerol; possible structure-based representation.



CAS has formulated policies for the indexing of dendrimers,[7] but only in ***textual*** terms; structures of these types of polymers are not currently indexed. Although many star-polymer references can be found by a search in file CA of the free-text phrase "star polymer or star polymers", as of October, 1997, CAS still had no official indexing policy for star polymer structures.

The International Union of Pure and Applied Chemistry (IUPAC) has recently addressed star and star-block polymer representations.[8,9] As of September, 1997, no specific recommendations on nomenclature or structure representation for dendrimers have been published.

This paper describes the systematic nomenclature and structural representation of dendritic, star, star-block, and star-branched polymers, and their registration in the DuPont SCION database. All examples given are theoretical and may or may not have been reduced to practice.

3. DENDRIMERS

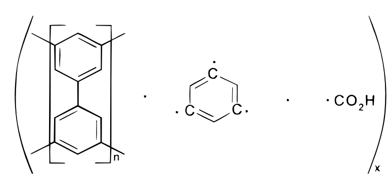
In SCION, dendrimers are considered to be hyperbranched polymers, and no distinction is currently made between dendrimers and other types of hyperbranched polymers. A hyperbranched or hypercross-linked polymer in SCION is defined as one in which at least one SRU or structure-based monomer unit has a connectivity greater than two. Whereas it may be difficult to determine whether cross-linking is present, and if so to what extent, there is little doubt about a hyperbranched structure in terms of the SRU(s) or monomer unit(s) that represent(s) the polymer. Because there is frequently uncertainty about whether a polymer designed to be hyperbranched is also cross-linked, the SCION controlled-term text descriptor used to identify these polymers is POLY-HYPERCONNECTABLE. This "combined concept" term circumvents the need to know, from a polymer registration point of view, whether a hyperbranched polymer is also cross-linked. The term POLY-HYPERCONNECTABLE implies that hyperbranching and/or hypercross-linking ***can*** occur because it refers to an SRU or monomer unit, although the descriptor is applied to the polymer containing that SRU or monomer unit. It implies that, based on the SRUs or monomers present, hyperbranching and/or hypercross-linking ***may*** occur during polymerization, not that it ***has*** occurred. In SCION, all polymers containing monomer units and/or SRUs with a connectivity of greater than two, except well-known types of conjugated monomers such as 1,3-butadiene, are identified by the text descriptor POLY-HYPERCONNECTABLE.

3.1. Structure-Based Registration of Dendrimers with Three Crossing Bonds. Because of CASRS limitations that apply to all SRUs with odd numbers of crossing bonds (3, 5, 7, etc.), dendrimers, whether symmetrical (e.g., A_3-type) or asymmetrical (e.g., AB_2-type), that are ideally represented as SRUs with three crossing bonds are currently unregistrable by structure-based methods.

To circumvent this problem, a symmetrical, A_3-type SRU, such as poly-1,3,5-benzenetriyl,[10] whether prepared as a dendrimer[11] or as a hyperbranched polymer,[12] is "doubled" to an A_4-type, such as poly-3,3′,5,5′-biphenyltetrayl (see Chart 1), which is registrable (see example 3.1.1a). Structure 3.1.1a is preferred to structure 3.1.1b.[13] Because of current software limitations, CAS can create neither the ideal representation, structure 3.1.1c, nor the hyperbranched representation, structure 3.1.1d. Registration as the ladder polymer structure 3.1.1a is a compromise.

When structures of end groups are known, they are registered (as fragments) as part of the overall polymer structure; the method is described elsewhere.[1,14] Thus, the polymer with an SRU shown as example 3.1.1c, peripheral carboxy groups, and a 1,3,5-benzenetriyl core is named and represented structurally (with appropriate fragments) as shown in example 3.1.2. The core is also called "end group" to avoid the need to create a separate word or phrase to describe it.

Example 3.1.2. POLY-3,3′,5,5′-BIPHENYLTETRAYL, END GROUP 1,3,5-BENZENETRIYL, END GROUP CARBOXY

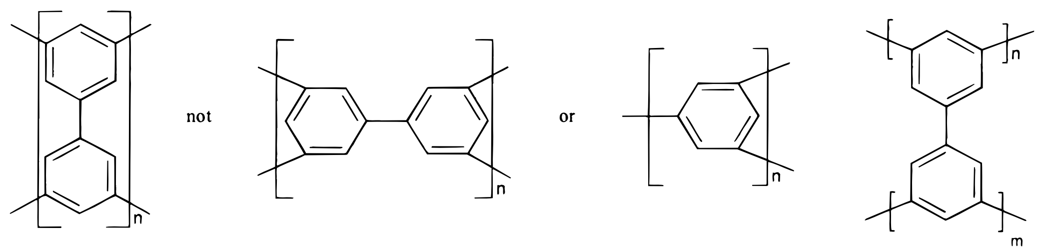


Note on example 3.1.2: A nomenclature system for multiple-radical fragments such as 1,3,5-BENZENETRIYL is described elsewhere.[14] This reference cites CAS Eighth Collective Index (8CI) nomenclature names, e.g. s-PHENENYL; names in the SCION chemical file are in the process of being updated to CAS Ninth Collective Index (9CI) nomenclature. Every polymer fragment, such as the carboxy and 1,3,5-benzenetriyl ones shown here, is registered with

Chart 1

Example 3.1.1. Poly-3,3′,5,5′-biphenyltetrayl

Example 3.1.1a. Example 3.1.1b. Example 3.1.1c. Example 3.1.1d.



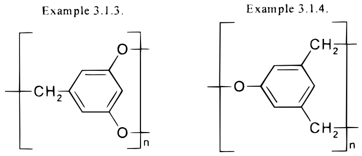
Polymer name: POLY-3,3′,5,5′-BIPHENYLTETRAYL
Text descriptors: POLY-HOMO; POLY-HYPERCONNECTABLE

an 8:DP,FRA textual descriptor to distinguish it from a true free radical; this is described in more detail elswehere.[1a]

The "doubling" solution fails for AB_2- and AB_3-type SRUs, and source-based methods have to be used. Strictly speaking, this should be discussed later under source-based dendrimers (section 3.3), but it is more convenient to deal with it here.

The situation is illustrated by two well-known dendritic structures, shown as examples 3.1.3 and 3.1.4, which should ideally both be registered with structure-based representations, but this is currently impossible because of CASRS limitations. Example 3.1.3 is the classical Fréchet dendritic wedge;[15] example 3.1.4, the "reverse" of example 3.1.3, was reported by Tyler and Hanson.[16]

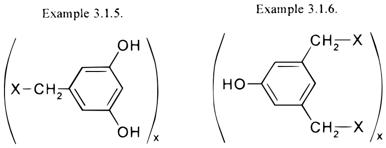
Example 3.1.3. Example 3.1.4.



Attempts to "double" these AB_2-types to give SRUs with even numbers of crossing bonds fail. Therefore, they have to be registered as source-based polymers (see examples 3.1.5 and 3.1.6).

Examples 3.1.5 and 3.1.6. Source-based registration of two special-case dendritic polymers (X = Br or OH).

Example 3.1.5. Example 3.1.6.



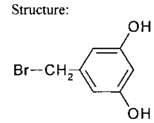
This source-based monomer unit approach creates a registration dilemma: whether to register the aliphatic alcohol, its corresponding bromide, or both. If only the bromide is registered, for example, a search designed to retrieve the aliphatic alcohol may fail to retrieve the bromide; the inverse situation is also true. If both are registered, a different problem arises in that intellectually the same polymer is registered with two separate structures and two registration numbers; this is prohibited by SCION polymer registration policy, principally because data (e.g., document references) to it will inevitably become scattered over time, and file integrity will therefore be compromised.

The current solution to this problem is to register all six substances [examples 3.1.3, 3.1.5 (X = Br), and 3.1.5 (X = OH); 3.1.4, 3.1.6 (X = Br), and 3.1.6 (X = OH)] with appropriate comments in the NOTES field of each registry record.[17]

The bromide and alcohol are registered as source-based substances, and the bromide is nominated as the polymer precursor. The AB_2-type SRU is registered with a name but no structure; although this offers the advantage that the SRU is named, and may therefore be retrieved by a name search, lack of structure is a disadvantage. It follows that polymers containing it also can have no structure representation for the SRU; because substructure searches cannot retrieve such substances, this approach is used only as a cross-reference in SCION. Polymers containing SRUs with structures such as 3.1.3 and 3.1.4 are registered with the corresponding source-based structures 3.1.5 and 3.1.6. Examples 3.1.7 through 3.1.9 show the records for the bromide, the alcohol, and the SRU, respectively.

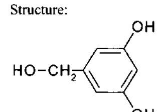
Example 3.1.7. Record for 3,5-dihydroxybenzyl bromide

CNUM: 1234A[18]
Name: 1,3-BENZENEDIOL, 5-(BROMOMETHYL)-
Synonyms: BENZYL BROMIDE, 3,5-DIHYDROXY-; 3,5-DIHYDROXYBENZYL BROMIDE; RESORCINOL, 5-(BROMOMETHYL)-
X-reference: CNUM 3456C
Notes: the source-based structure $(C_7H_7BrO_2)_x$ is used for source-based representation of the poly(oxymethylene-1,3,5-benzenetriyl) SRU $(C_7H_5O)_n$, CNUM 3456C, and copolymers therefrom.
Structure:



Example 3.1.8. Record for 3,5-dihydroxybenzyl alcohol

CNUM: 2345B
Name: 1,3-BENZENEDIOL, 5-(HYDROXYMETHYL)-
Synonyms: BENZYL ALCOHOL, 3,5-DIHYDROXY-; 3,5-DIHYDROXYBENZYL ALCOHOL; RESORCINOL, 5-(HYDROXYMETHYL)-
Notes: poly(oxymethylene-1,3,5-benzenetriyl) SRU, and polymers containing it, are registered as if they were prepared from 3,5-dihydroxybenzyl bromide (CNUM 1234A).
MF: $C_7H_8O_3$
Structure:



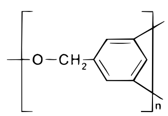
Example 3.1.9. Cross-reference for AB_2-type SRU shown as example 3.1.3

CNUM: 3456C
Polymer name: POLY(OXYMETHYLENE-1,3,5-BENZENETRIYL)
MF: $(C_7H_5O)_n$
Structure: none
X-reference: CNUM 1234A
Notes: see CNUM 1234A for source-based representation; polymers with this SRU contain 1234A as a (co)monomer unit.

Notice that the SRU contains a "phase shift", which is discussed later.

SCION nomenclature rules[19] have been modified by the addition of two new rules (see *Appendix*) to handle SRUs with unequal numbers of left- and right-crossing bonds, such as AB_2- and AB_3-types, so that the convention used in most publications on dendrimers is preserved; representations are drawn with the A bond on the left and the B bonds on the right. However, application of these new rules results in a "phase shift"; that is, a movement of the left- and right-limiting parentheses along the chain to redefine the SRU. Thus, the SRU, as originally drawn by Fréchet[15] (see example 3.1.3), is phase-shifted to the "minimum-atom" configuration shown as example 3.1.10. Notice that the name given in example 3.1.9 corresponds to the phase-shifted structure of example 3.1.10, ***not*** to the original Fréchet structure.

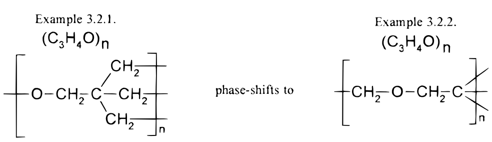
Example 3.1.10. Phase-shifted, minimum-atom configuration for the Fréchet wedge SRU.



Searchers who retrieve the name of the SRU are thus steered to the bromide, CNUM 1234A, (see example 3.1.7) and polymers therefrom.

3.2. Structure-Based Registration of Dendrimers with Four Crossing Bonds. The CASRS is capable of registering AB_3-type SRUs, but the on-screen image displayed is non-standard. Thus, for the AB_3-type SRU shown as example 3.2.1, the image on terminals with graphics capabilities appears with black dots for the carbon atoms and a white dot for the oxygen atom. The image on text-type terminals is also hard to interpret.

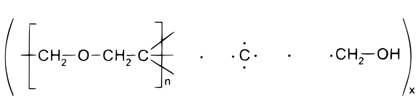
Examples 3.2.1 and 3.2.2. The AB_3-type SRU "poly-(oxyneopentanetetrayl)", example 3.2.1, is registered as the phase-shifted structure of example 3.2.2.



Polymer name: POLY-METHYLENEOXY-1-ETHANYL-2-YLIDYNE[20]
Text descriptors: POLY-HOMO; POLY-HYPERCONNECTABLE

This "Starburst" polymer, prepared from pentaerythritol and a bicyclic ether by a multi-step process,[21] has outer (terminal) hydroxy groups. Example 3.2.3 shows its registration in SCION.

Example 3.2.3. Registration in SCION of "Starburst" dendrimers such as PE-OH(36), PE-OH(108), etc.

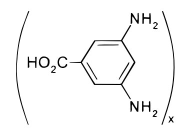


Polymer name: POLY-METHYLENEOXY-1-ETHANYL-2-YLIDYNE, END GROUP HYDROXYMETHYL, END GROUP METHANETETRAYL
Text descriptors: POLY-HOMO; POLY-HYPERCONNECTABLE
Notes on example 3.2.3: (1) PE-OH(36) is $C[CH_2OCH_2C[CH_2OCH_2C(CH_2OH)_3]_3]_4$; PE-OH(108) is the next generation. (2) Nomenclature for multiradicals such as methanetetrayl (shown in this polymer name) is described elsewhere.[14]

Currently it is the policy of both CAS and DuPont not to register the same polymer with different molecular weights as separate substances with different registration numbers. This policy means that different dendritic generations in SCION are currently indistinguishable from one another. Thus, "Starburst" dendrimers PE-OH(36) and PE-OH(108), both of which qualify as polymers because the number of repeat units is >10, receive the same SCION CNUM. Should the registration policy change, a unique special input text descriptor[22] could be added to enable registration of different dendrimer generations.

3.3. Source-Based Registration of Dendrimers. Source-based registration in SCION of AB_2-types, AB_3-types, etc. follows the general principles for source-based registration of linear single-strand polymers;[1] prescribed monomer condensation (PMC) polymers (as defined in a 1995 paper[1] and summarized in the note following example 3.3.1) are ***never*** registered in SCION as SRUs. Example 3.3.1 illustrates the method for the AB_2-type 3,5-diaminobenzoic acid.

Example 3.3.1. Source-based registration of polymer from 3,5-diaminobenzoic acid (DABA).

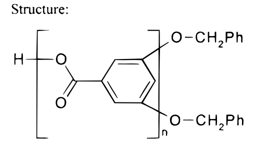


Polymer name: POLYAMIDE-BENZOIC ACID, 3,5-DIAMINO-
Text descriptors: POLYAMIDE; POLY-HOMO; POLY-HYPERCONNECTABLE

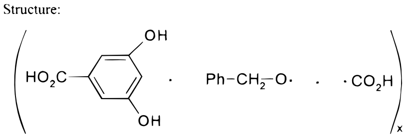
Note on example 3.3.1: SCION structures of PMC polymer classes—polyamides (PA), polycarbonates (PC), polyesters (PE), polyimides (PI), polyureas (PR), polyurethanes (PU), and combinations of these six—are registered with stylized source-based monomer units, which are not necessarily the actual monomer units; thus, this polymer is registered with DABA as the stylized monomer unit regardless of whether the actual monomer unit is DABA or a simple derivative (e.g., its ethyl ester).[1] A 1995 paper[1] described only PMC classes PA, PE, PI, PU, and their combinations; the list has now been expanded to include PCs, PRs, and their combinations.

Examples 3.3.2, 3.3.3, and 3.3.4, respectively, show the monodendron from 3,5-dihydroxybenzoic acid with benzyl peripheral groups, its source-based representation (from 3,5-dihydroxybenzoic acid with benzyl peripheral groups and a carboxy attachment point), and the dendrimer prepared from it and 4,4′,4″-ethylidynetriphenol.[23]

Example 3.3.2. Idealized monodendron from 3,5-dihydroxybenzoic acid
Structure:



Example 3.3.3. SCION representation of the monodendron from 3,5-dihydroxybenzoic acid
Structure:



Polymer name: POLYESTER-BENZOIC ACID, 3,5-DIHYDROXY-, END GROUP CARBOXY, END GROUP PHENYLMETHOXY
Text descriptors: POLYESTER; POLY-HOMO; POLY-HYPERCONNECTABLE

There is no indication of how many end groups of each type there are; however, the overall monodendron structure is readily deducible from the name and structural components. Each end group, with its ***complete*** functionality, is

Chart 2. Preparation of a PAMAM from Ammonia, Methyl Acrylate, and Ethylenediamine

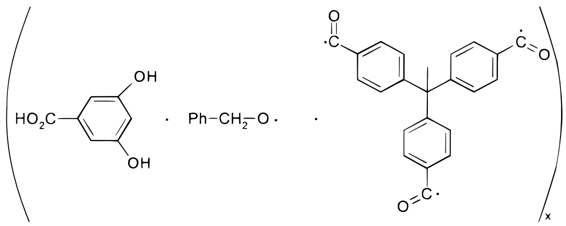
Step 1. NH_3 + 3 CH_2=CH-CO_2Me -> N($CH_2CH_2CO_2$Me)$_3$ (I)

Step 2. (I) + (excess) $H_2NCH_2CH_2NH_2$ -> N($CH_2CH_2CONHCH_2CH_2NH_2$)$_3$ (II) (first generation)

Step 3. (II) + 3 CH_2=CH-CO_2Me -> N[$CH_2CH_2CONHCH_2CH_2$N($CH_2CH_2CO_2$Me)$_2$]$_3$ (III)

Step 4. (III) + (excess) $H_2NCH_2CH_2NH_2$ ->
N[$CH_2CH_2CONHCH_2CH_2$N($CH_2CH_2CONHCH_2CH_2NH_2$)$_2$]$_3$ (IV) (second generation)
etc.

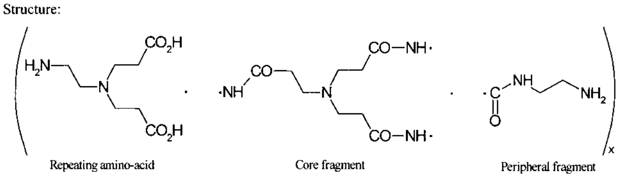
named;[1] a systematic nomenclature system for such multiradicals is described elsewhere.[14]



Polymer name: POLYESTER-BENZOIC ACID, 3,5-DIHYDROXY-, END GROUP ETHYLIDYNETRIS(1,4-PHENYLENEOXYCARBONYL) END GROUP PHENYLMETHOXY
Text descriptors: END GROUP, MULTICHAIN; POLYESTER; POLY-HOMO; POLY-HYPERCONNECTABLE

Example 3.3.5 shows how a typical Tomalia poly(amidoamine) ("PAMAM") dendrimer[2b] is registered in SCION. The stepwise preparation, illustrated in Chart 2, never involves an amide condensation, but because the product is in fact a polyamide it is registered in SCION in terms of (1) the single theoretical parent amino-acid and (2) the core- and peripheral-group fragments that constitute the rest of the polymer. Note that the fragment structures are derived in relation to the theoretical amino-acid that constitutes the repeating unit, not to the true ammonia (NH_3) core and the amino (-NH_2) end groups described by Tomalia. In terms of the theoretical amino-acid parent, it is a homopolymer. The real reactants are, of course, registered in the bibliographic file of SCION, but are ***not*** part of the chemical-file polymer record.

Example 3.3.5. SCION record for the PAMAM of structure (IV) (see chart 2)
Structure:



Polymer name: POLYAMIDE-PROPANOIC ACID, 3,3′-((2-AMINOETHYL)IMINO)BIS-, END GROUP (((2-AMINOETHYL)AMINO)CARBONYL, END GROUP NITRILOTRIS(1,2-ETHANEDIYLCARBONYLIMINO)
Text descriptors: END GROUP, MULTICHAIN; POLYAMIDE; POLY-HOMO; POLY-HYPERCONNECTABLE

4. STAR, STAR-BLOCK, AND STAR-BRANCHED POLYMERS

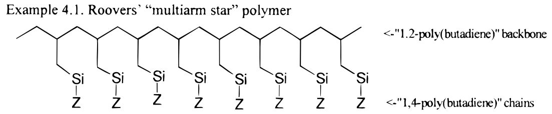
The terms "star polymer", "star-shaped polymer", and "star-block polymer" are used imprecisely in the published literature to describe at least three physically different star polymer types. IUPAC defines a star polymer as "a polymer composed of star macromolecules", and a star macromolecule as "a macromolecule containing a single branch point from which linear chains (arms) emanate".[24] As of October, 1997, IUPAC has published no terminology for polymers containing linear or branched arms and polymeric or non-polymeric, multi-atomic centers or cores.

To date, every star polymer encountered in SCION falls into one of two well-defined categories, which are described in this paper.

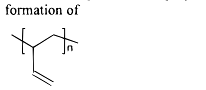
Category A. Category A includes polymers comprising a precise, **non**-polymeric center or core of known structure, from which radiate a known number of arms. The core moiety may be acyclic (e.g., 1,2,3,4,5,6-hexanehexayl) or cyclic (e.g., 1,2,3,4,5,6-cyclohexanehexayl) (see point 1).

Point 1. If the center is itself polymeric and linear (i.e., not dendritic or hyperbranched), the polymer is considered in SCION to be a comb or graft polymer, rather than a star polymer; in contrast, Roovers *et al.*[25] call such a polymer a "multiarm star" (see example 4.1).

Example 4.1. Roovers' "multiarm star" polymer



Note on example 4.1: "1,2-polybutadiene" means 1,3-butadiene polymerized in the "1,2" mode, i.e. formation of



"1,4-polybutadiene" means 1,3-butadiene polymerized in the "1,4" mode, i.e. formation of (-C-C=C-C-)$_n$.

Category B. Category B includes polymers comprising a polymeric core from which a number of arms emanate; the core may be either dendritic or hyperbranched, and the number of arms may be known (as is frequently the case with dendritic cores) or unknown (as is usually the case with hyperbranched cores).

For both of these categories, each arm may be built from one SRU or monomer unit ("homopolymeric" arm), or each may be a random, statistical, or block copolymer; star polymers containing "blocky"[26] arms are usually called "star-block polymers". Each arm may be completely linear, or it may contain branching that is introduced at intervals to increase the number of linear segments (see example 2.1).

Star polymers containing a hyperbranched center are often called "star-branched polymers".[27]

Structure representation in SCION for both categories A and B is based on one or more SRUs (i.e., structure-based), one or more component monomer units (i.e., source-based), or a combination of both. The categories and types of structure-based star polymers in SCION are summarized in Table 1. Each of these is discussed in more detail in sections 4.3 and 4.4, and examples are given.

4.1. Rules for Nomenclature of Star Polymers. Star polymers in SCION can be represented by the general format shown as example 4.1.1.

Table 1. Classification of Star Polymers in SCION

category & type	core[a]	arm/arm relationship[b]	monomer unit or SRU types per arm[c]	structure of each arm
A-1	non-polymeric	identical	1	homo,[d] linear[e]
A-2	non-polymeric	identical	>1	ran./stat.,[f] linear
A-3	non-polymeric	identical	>1	ran./stat., branched[e]
A-4	non-polymeric	identical	>1	block,[g] linear
A-5	non-polymeric	identical	>1	block, branched
A-6	non-polymeric	nonidentical	1	homo, linear
A-7	non-polymeric	nonidentical	>1	ran./stat., linear
A-8	non-polymeric	nonidentical	>1	ran./stat., branched
A-9	non-polymeric	nonidentical	>1	block, linear
A-10	non-polymeric	nonidentical	>1	block, branched
B-1	polymeric	identical	1	homo, linear
B-2	polymeric	identical	>1	ran./stat., linear
B-3	polymeric	identical	>1	ran./stat., branched
B-4	polymeric	identical	>1	block, linear
B-5	polymeric	identical	>1	block, branched
B-6	polymeric	nonidentical	1	homo, linear
B-7	polymeric	nonidentical	>1	ran./stat., linear
B-8	polymeric	nonidentical	>1	ran./stat., branched
B-9	polymeric	nonidentical	>1	block, linear
B-10	polymeric	nonidentical	>1	block, branched

[a] "Polymeric" includes both dendritic and hyperbranched cores; currently no distinction is made between these types in SCION. [b] "Identical" means that all arms are identical with one another with respect to the SRU(s) or monomer unit(s) contained therein, but not necessarily with respect to arm length and/or the precise monomer or SRU sequence or orientation within the arms. "Nonidentical" means that there are at least two different types of arm present with regard to the monomer unit(s) or SRU(s) contained therein. Thus, a three-arm star may have one arm of one type and two of another, or all three arms may be different. [c] For category B polymers with nonidentical arms, these are the minimum requirements. Thus, a polymer qualifies for the descriptor POLY-BLOCK as long as at least one type of arm is "blocky". However, polymers with homo arms qualify for the descriptor POLY-HOMO only when ***all*** arms, whether identical or dissimilar, comprise homopolymers; polymers with homopolymer arms and "blocky" or ran./stat. arms do not qualify for the descriptor POLY-HOMO. [d] "Homo" means that each arm independently may comprise head-to-head (hh) units only, head-to-tail (ht) units only, or "either/unknown" (eu), where this is possible with only one SRU or monomer unit; for example, the oxypropylene SRU is written formally in SCION as $(\text{-O-CH(CH}_3\text{)-CH}_2\text{-})_n$, but in practice within poly(oxypropylene) strings it may exist as mixed $(\text{-O-CH(CH}_3\text{)-CH}_2\text{-})_n$ and $(\text{-O-CH}_2\text{-CH(CH}_3\text{)-})_n$. Similarly, styrene units may be oriented hh, ht, or eu. [e] "Linear" means that each arm comprises one single strand. "Branched" means that each arm contains at least one branch point within its length, but that the branching monomer unit(s) or SRU(s) is/are not the only monomer unit(s) or SRU(s) in the arm. Therefore, this excludes arms in which ***every*** monomer unit or SRU is branched; such arms constitute monodendrons, and polymers containing this type of arm are classified in SCION as dendrimers or hyperbranched polymers, not as star polymers (see section 3). [f] "Ran./stat." means that each arm comprises two or more SRUs or monomer units joined in a random or statistical manner by polymerization. [g] "Block" means that each arm is "blocky".

Example 4.1.1. General format for a SCION star polymer.

core/nucleus — repeating entity/ies — peripheral end groups

The following general rules apply to all star polymers discussed in this paper:

1. The repeating entity/ies is/are named.
2. The core/nucleus and peripheral end groups are named whenever they are identified in source documents. In simpler star polymers with a non-polymeric center, the non-repeating center moiety is usually described as the "core"; in more complex star polymers with a dendritic center, the word "nucleus" is used in this paper to describe the non-repeating center moiety because the word "core" is ambiguous in that it usually refers to the whole central dendrimer.
3. The polymer name is assembled to read: PREFIX-REPEATING_ENTITY/IES, END GROUP A, END GROUP B in which the A end group alphabetically precedes the B end group in the final name, regardless of which is the core/nucleus and which is the peripheral end group.

Each part of the polymer is named according to previously published rules for polymers in SCION.[1] Each part is described below.

Prefix. For PMC polymers, the prefix identifies the polymer class (e.g., POLYAMIDE-, POLYAMIDE-ESTER-, POLYAMIDE-ESTER-URETHANE-). For ASM (actual starting material[1]) source-based polymers and SRUs, the prefix is simply POLY-.

Repeating Entity/ies. Category 1 (PMC): source-based monomer units are named by their stylized names (e.g., BENZOIC ACID, 3,5-DIAMINO).[1] Category 2 (ASM): source-based monomer units are named by their actual names (e.g., 2-PROPENOIC ACID, 1,2-ETHANEDIYL ESTER).[1] Category 3 (SRU): SRUs are named according to SCION rules for SRU nomenclature[1,19] (see also *Appendix* to this paper. As explained in detail elsewhere,[1] multicategory polymers contain the word WITH in the name; category 1 entities have highest priority in a name, followed in turn by categories 2 and 3 (see example 4.1.2.).

Example 4.1.2. POLYAMIDE-BENZOIC ACID, 4-DI-AMINO- WITH POLY-OXY-1,2-ETHANEDIYL

Modifers such as ALTERNATING, BLOCK, STAR, etc., that describe the nature of the polymer are generally added after citation of all the repeating entities and before citation of end groups (see example 4.1.3).

Example 4.1.3. POLY-2-PROPENOIC ACID, BUTYL ESTER/2-PROPENOIC ACID, METHYL ESTER, BLOCK.

In multilevel polymers,[28] when appropriate, a modifier such as BLOCK is moved from its normal position in the name to a location such that the precise nature of the blockiness is indicated. Thus, the position of the word BLOCK in example 4.1.4 indicates very clearly that a poly-oxyethylene/oxypropylene block macrodiol is used.

Example 4.1.4. POLYESTER-1,4-BENZENEDIOIC ACID/(POLY-OXY-1,2-ETHANEDIYL/OXY-(1-METHYL-1,2-ETHANEDIYL), BLOCK)/1,3-PROPANEDIOL

In keeping with IUPAC recommendations that the word "variegated" be used to describe star polymers with non-identical arms,[8] the word VARIEGATED is added as a text descriptor (but not as part of the name) for polymers with different monomer units or SRUs in different arms. There is currently indication of neither how many arms contain one type of source-based monomer unit or SRU "homopolymer" and how many contain another, nor which end groups are attached to which arms. However, such information could be added in the form of one or more text descriptors, or as a free-text explanation in the NOTES field.

For star-branch polymers, there is no indication of the degree of arm branching (i.e., information on the percentage of branching monomer unit or SRU is not part of the polymer record); nor is there any information as to where in the linear chains the branching units are situated.

End Groups. The core/nucleus and peripheral end groups are named and alphabetized, regardless of which is which (see example 4.1.5).

Example 4.1.5. POLY-OXY-1,2-ETHANEDIYL, END GROUP ACETYLOXY, END GROUP 1,2,3,4,5,6-HEXANEHEXAYLHEXAOXY

Note on example 4.1.5: There is a structural inconsistency in this and other examples in this paper; the SRU and fragments do not "fit together" to give the complete polymer - in this example there are additional oxygen atoms. This inconsistency is because SCION nomenclature rules dictate that each ***complete*** end group shall be named and structured. Thus, in polyethylene glycol, functionally speaking, there are two hydroxy groups, not one hydro group and one hydroxy group. This concept is discussed in more detail elsewhere.[1b]

In cases where alternative peripheral end groups are possible, they are named, alphabetized, and separated by slashes; in such cases, the alternative end group name cluster is alphabetized as a single unit so that the concept of alternate peripheral end groups cannot be split by insertion of the name of the core/nucleus end group. Thus, in a star polymer with either carboxy or hydroxy peripheral end groups, the name cluster CARBOXY/HYDROXY in the expression END GROUP CARBOXY/HYDROXY is alphabetized on CARBOXY (see example 4.1.6).

Example 4.1.6. POLYESTER-1,2-ETHANEDIOL/HEXANEDIOIC ACID, STAR, END GROUP 1,3,5-BENZENETRIYLTRIS(CARBONYLOXY), END GROUP CARBOXY/HYDROXY

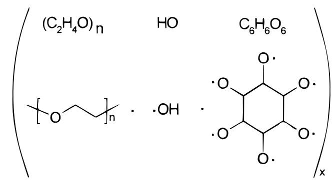
4.2. Registration of Star Polymers in SCION. Sections 4.3 and 4.4 give examples of how different star polymers are registered. Structures and names are given, and text descriptors such as POLY-BLOCK, POLY-HYPERCONNECTABLE, POLY-STAR, etc. are added as appropriate. Points of interest for some of the examples that are not covered by the general description in section 4.1 are added as necessary.

4.3. Category A Star Polymers. In category A, the center of the polymer is a ***non***-polymeric, multiply bonded moiety (e.g., 1,2,3,4,5,6-cyclohexanehexayl, silanetetrayl, 1,3,5-benzenetriyl, etc.). The moiety structure and number of connections are known precisely.

Category A-1. All linear arms are identical (see note b under Table 1); each contains only one type of source-based monomer unit or SRU.

Example 4.3.1. Star polymer from 1,2,3,4,5,6-cyclohexanehexol and oxirane.

Special input text descriptor: 8:DP,STA[22]
Structure:

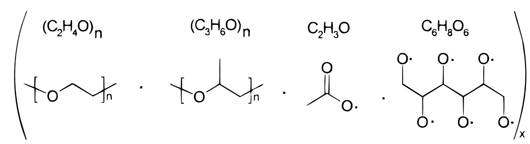


Polymer name: POLY-OXY-1,2-ETHANEDIYL, STAR, END GROUP 1,2,3,4,5,6-CYCLOHEXANEHEXAYLHEXAOXY, END GROUP HYDROXY
Text descriptors: END GROUP, MULTICHAIN; POLY-STAR

Category A-2. All linear arms are identical (see note b under Table 1); each is composed of at least two types of source-based monomer unit or SRU, with the monomer units or SRUs arranged randomly or statistically.

Example 4.3.2. Star polymer from 1,2,3,4,5,6-hexanehexol from methyloxirane and oxirane; peripheral hydroxy groups are acetylated.

Special input text descriptor: 8:DP,STA
Structure:

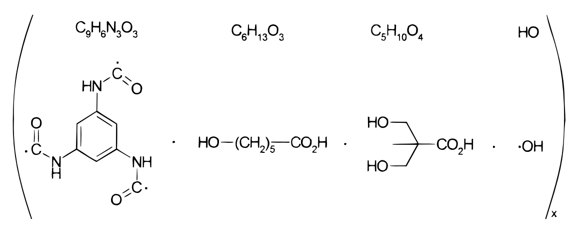


Polymer name: POLY-OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), STAR, END GROUP ACETYLOXY, END GROUP 1,2,3,4,5,6-HEXANEHEXAYLHEXAOXY
Text descriptors: POLY-STAR; END GROUP, MULTICHAIN

Category A-3. All arms are identical (see note b under Table 1); each arm contains at least two types of source-based monomer unit or SRU. At least one type of monomer unit or SRU has a connectivity of two, and at least one type of monomer unit or SRU is branched (i.e., it has a connectivity of more than two).

Example 4.3.3. Star polymer with a 1,3,5-benzenetriamine core and three branched arms each comprising a copolymer of 6-hydroxyhexanoic acid (linear source-based monomer unit) and 2,2-bis(hydroxymethyl)propionic acid (branching source-based monomer unit).

Special input text descriptor: 8:DP,STA
Structure:

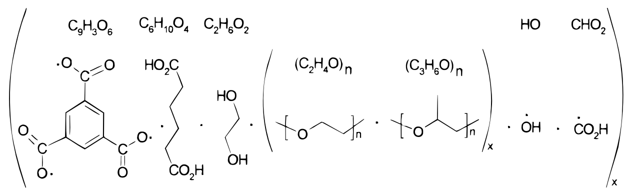


Polymer name: POLYESTER-HEXANOIC ACID, 6-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-2-(HYDROXYMETHYL)-2-METHYL-, STAR, END GROUP 1,3,5-BENZENETRIYLTRIS(IMINOCARBONYL), END GROUP HYDROXY
Text descriptors: POLYESTER; POLY-STAR; POLY-HYPERCONNECTABLE

Category A-4. All linear arms are identical (see note b under Table 1) and each arm is "blocky".

Example 4.3.4.1. Star polymer with a 1,3,5-benzenetricarboxylic acid core and three "blocky" arms comprising adipic acid/ethylene glycol polyester segments and randomly connected poly-oxyethylene/oxypropylene SRU segments (compare with example 4.3.4.2).

Special input text descriptor: 8:DP,STA
Structure:

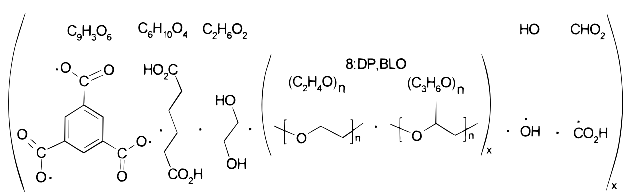


Polymer name: POLYESTER-1,2-ETHANEDIOL/HEXANEDIOIC ACID WITH (POLY-OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL)), STAR, END GROUP 1,3,5-BENZENETRIYLTRIS(CARBONYLOXY), END GROUP CARBOXY/HYDROXY
Text descriptors: POLYESTER; POLY-MULTICATEGORY; POLY-MULTILEVEL; POLY-STAR

Notes on example 4.3.4.1: (1) Although this is a star-block polymer, it does not qualify in SCION for the text descriptor POLY-BLOCK or addition of the word BLOCK in the polymer name. Separation of the monomer unit names from the SRU names in the complete polymer name by use of the word "WITH" implies blockiness, and the text descriptor POLY-MULTICATEGORY is used to indicate the presence in this polymer name of source-based name segments and structure-based name segments.[1c] (2) "Multicategory" in the sense used in the text descriptor POLY-MULTICATEGORY refers not to categories of star polymers discussed in this paper, but to the three broad categories of polymers in SCION - PMC, ASM, and SRU.[1] (3) As with all star polymers in SCION, the polymer is registered with addition of a special input text descriptor that includes STA to denote a star polymer. (4) The poly-oxyethylene/oxypropylene SRU segments comprise a macrodiol, which is a polymer in its own right; incorporation of this into a larger polymer means that the star polymer is a multilevel polymer; hence the descriptor POLY-MULTILEVEL and use of two sets of brackets. Multilevel polymer registration was described recently.[28]

Example 4.3.4.2. Star-block polymer with a 1,3,5-benzenetricarboxylic acid core and three "blocky" arms comprising adipic acid/ethylene glycol polyester segments and poly-oxyethylene/oxypropylene SRU block-copolymer segments (compare with example 4.3.4.1).

Special text descriptor: 8:DP,STA
Structure:



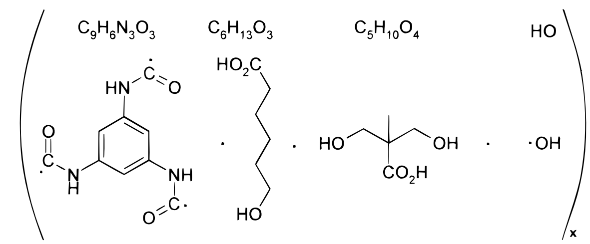
Polymer name: POLYESTER-1,2-ETHANEDIOL/HEXANEDIOIC ACID WITH (POLY-OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), BLOCK), STAR, END GROUP 1,3,5-BENZENETRIYLTRIS(CARBONYLOXY), END GROUP CARBOXY/HYDROXY
Text descriptors: POLYESTER; POLY-BLOCK; POLY-MULTICATEGORY; POLY-MULTILEVEL; POLY-STAR

Notes on example 4.3.4.2: The individual structural components of this polymer are identical with those of example 4.3.4.1, and the overall polymer is registered with the same special input text descriptor, namely 8:DP,STA. However, this polymer is different from the previous example because the intermediate poly-oxyethylene/oxypropylene macrodiol in this polymer is a block polymer that is registered with the text descriptor 8:DP,BLO to distinguish it from its random counterpart in example 4.3.4.1. This is sufficient to impart uniqueness to this star polymer. The special input text descriptor[22] BLO indicates a block polymer.

Category A-5. All arms are identical (see note b under Table 1); each arm contains at least two types of source-based monomer unit or SRU. At least one type of monomer unit or SRU has a connectivity of two, and at least one type of monomer unit or SRU is branched (i.e., it has a connectivity of more than two). The polymer also contains block segments.

Example 4.3.5. Block-star polymer with a 1,3,5-benzenetriamine core and three "blocky", branched arms each comprising blocks of 6-hydroxyhexanoic acid (linear source-based monomer unit) and 2,2-bis(hydroxymethyl)propionic acid (branching source-based monomer unit).

Special input text descriptor: 8:DP,BLO,STA
Structure:

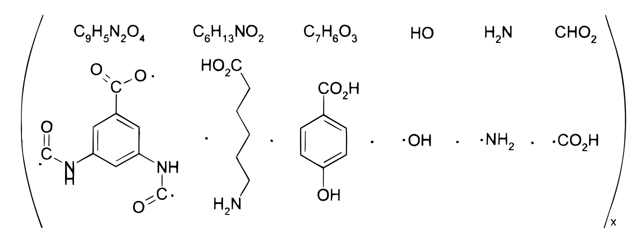


Polymer name: POLYESTER-HEXANOIC ACID, 6-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-2-(HYDROXYMETHYL)-2-METHYL-, BLOCK, STAR, END GROUP 1,3,5-BENZENETRIYLTRIS(IMINOCARBONYL), END GROUP HYDROXY
Text descriptors: POLYESTER; POLY-BLOCK; POLY-HYPERCONNECTABLE; POLY-STAR

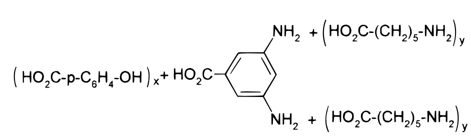
Category A-6. Each arm *per se* is a linear homopolymer; the composition of at least one arm differs from the others (see note b under Table 1).

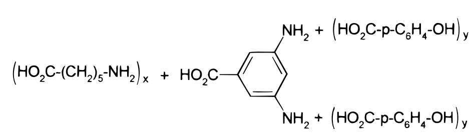
Example 4.3.6. Polyamide-ester from a 3,5-diaminobenzoic acid core, caprolactam (represented as the stylized monomer unit 6-aminohexanoic acid[1]), and *p*-hydroxybenzoic acid.

Special input text descriptor: 8:DP,STA,VAR
Structure:



Polymer name: POLYAMIDE-ESTER-BENZOIC ACID, 4-HYDROXY-/HEXANOIC ACID, 6-AMINO-, STAR, END GROUP AMINO/HYDROXY, END GROUP CARBOXY, END GROUP OXYCARBONYL-1,3,5-BENZENETRIYL-3-(IMINOCARBONYL)-5-(IMINOCARBONYL)
Text descriptors: END GROUP, MULTICHAIN; POLYAMIDE-ESTER; POLY-STAR; POLY-VARIEGATED
Note on example 4.3.6: The given name and structure cover two possibilities:



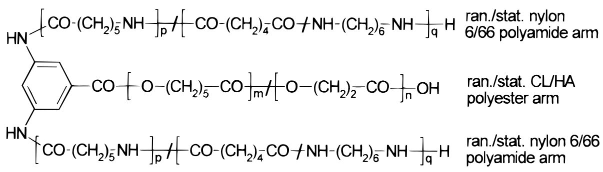


Thus, CARBOXY is an end group in both cases, but AMINO and HYDROXY are mutually exclusive alternatives and are therefore cited in the style END GROUP AMINO/HYDROXY.

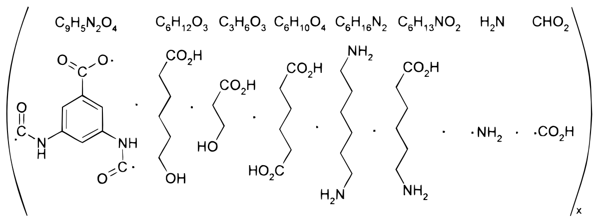
Category A-7. The composition of at least one arm differs from the others (see note b under Table 1); each arm *per se* is a linear random (or statistical) copolymer.

Example 4.3.7. Random/statistical polyamide-ester from a 3,5-diaminobenzoic acid core, adipic acid, caprolactam, caprolactone (CL), 1,6-hexanediamine, and hydracrylic acid (HA).

Idealized structure representation:



Special input text descriptor: 8:DP,STA,VAR
Stored structure:

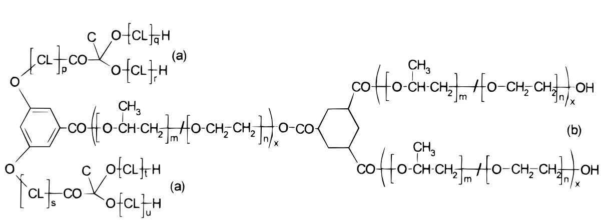


Polymer name: POLYAMIDE-ESTER-1,6-HEXANEDIAMINE/HEXANEDIOIC ACID/HEXANOIC ACID, 6-AMINO-/HEXANOIC ACID, 6-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-, STAR, END GROUP AMINO, END GROUP CARBOXY, END GROUP OXYCARBONYL-1,3,5-BENZENETRIYL-3-(IMINOCARBONYL)-5-(IMINOCARBONYL)
Text descriptors: END GROUP, MULTICHAIN; POLYAMIDE-ESTER; POLY-STAR; POLY-VARIEGATED

Note on example 4.3.7: Although this is a block polymer in the sense that the core moiety, which is functioning as a non-polymeric junction point, separates polyamide arms from polyester arms, this type is ***not*** considered in SCION to be a block polymer; for a polymer to be classified as a block polymer, the arms themselves must be "blocky".

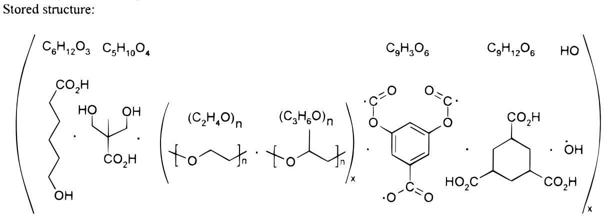
Category A-8. The composition of at least one arm differs from the others (see note b under Table 1); each arm *per se* is a random (or statistical) copolymer. At least one type of branching monomer unit or SRU is also present, and each of the otherwise linear arms therefore contains branch points.

Example 4.3.8. Branched star polyether-ester from a 3,5-dihydroxybenzoic acid core, an ethylene oxide/propylene oxide macrodiol, caprolactone (CL), 2,2-bis(hydroxymethyl)-propionic acid (HMPA) branching monomer unit, and 1,3,5-cyclohexanetricarboxylic acid (CHTA) branching monomer unit.



CL = the SRU from caprolactone, namely -(CO-(CH$_2$)$_5$-O-)$_n$-
(a) = linear CL arms with some HMPA branching
(b) = linear PEO/PPO macrodiol chain arms with some CHTA branching

Special input text descriptor: 8:DP,STA,VAR
Stored structure:

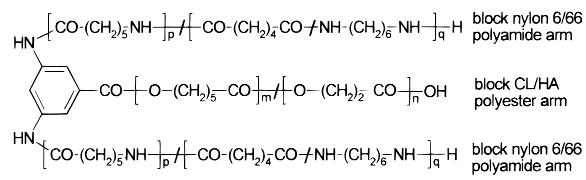


Polymer name: POLYESTER-1,3,5-CYCLOHEXANETRICARBOXYLIC ACID/HEXANOIC ACID, 6-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-2-(HYDROXYMETHYL)-2-METHYL- WITH (POLY-OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), STAR, END GROUP HYDROXY, END GROUP OXYCARBONYL-1,3,5-BENZENETRIYL-3-(OXYCARBONYL)-5-(OXYCARBONYL)
Text descriptors: END GROUP, MULTICHAIN; POLYESTER; POLY-MULTILEVEL; POLY-MULTICATEGORY; POLY-STAR; POLY-VARIEGATED

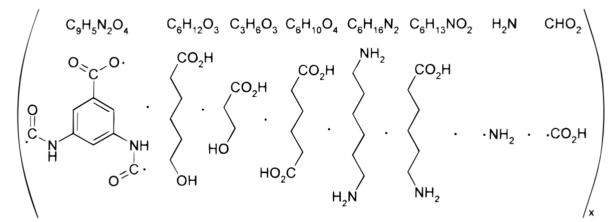
Category A-9. The composition of at least one arm differs from the others (see note b under Table 1); each arm *per se* is linear and "blocky".

Example 4.3.9. Block polyamide-ester from a 3,5-diaminobenzoic acid core, adipic acid, caprolactam, caprolactone (CL), 1,6-hexanediamine, and hydracrylic acid (HA) (this example differs from example 4.3.7 only in that the arms are "blocky").

Idealized structure representation:



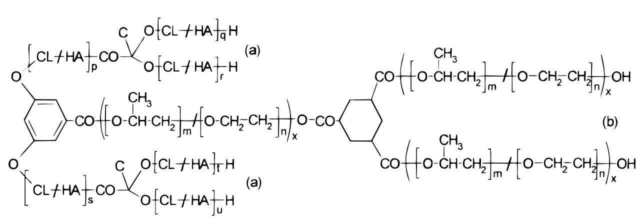
Special input text descriptor: 8:DP,BLO,STA,VAR
Stored structure:



Polymer name: POLYAMIDE-ESTER-1,6-HEXANEDIAMINE/HEXANEDIOIC ACID/HEXANOIC ACID, 6-AMINO-/HEXANOIC ACID, 6-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-, BLOCK, STAR, END GROUP AMINO, END GROUP CARBOXY, END GROUP OXYCARBONYL-1,3,5-BENZENETRIYL-3-(IMINOCARBONYL)-5-(IMINOCARBONYL)
Text descriptors: END GROUP, MULTICHAIN; POLYAMIDE-ESTER; POLY-BLOCK; POLY-STAR; POLY-VARIEGATED

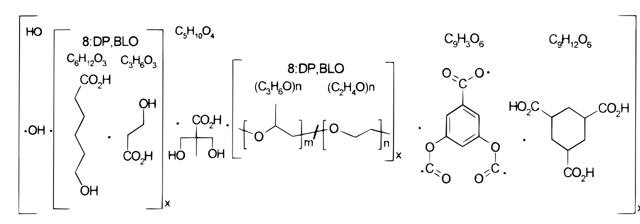
Category A-10. The composition of at least one arm differs from the others (see note b under Table 1); each arm *per se* contains some "blockiness" and at least one type of branching monomer unit or SRU.

Example 4.3.10. Branched star polyether-ester from a 3,5-dihydroxybenzoic acid core, an ethylene oxide/propylene oxide block macrodiol, caprolactone (CL)/hydracrylic acid (HA) block ester, 2,2-bis(hydroxymethyl)propionic acid (HMPA) branching monomer unit, and 1,3,5-cyclohexane-tricarboxylic acid (CHTA) branching monomer unit.



(a) = linear, "blocky" CL/HA arms with some HMPA branching
(b) = linear PEO/PPO block macrodiol arms with some CHTA branching

Special input text descriptor: 8:DP,STA,VAR
Stored structure:



Polymer name: POLYESTER-1,3,5-CYCLOHEXANETRICARBOXYLIC ACID/(HEXANOIC ACID, 6-HYDROXY-/PROPANOIC ACID, 3-HYDROXY, BLOCK)/PROPANOIC ACID, 3-HYDROXY-2-(HYDROXYMETHYL)-2-METHYL- WITH (POLY-OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), BLOCK), STAR, END GROUP HYDROXY, END GROUP OXYCARBONYL-1,3,5-BENZENETRIYL-3-(OXYCARBONYL)-5-(OXYCARBONYL)
Text descriptors: END GROUP, MULTICHAIN; POLY-BLOCK; POLYESTER; POLY-MULTICATEGORY; POLY-STAR; POLY-VARIEGATED

Note on example 4.3.10: Owing to space limitations in the ISIS/Draw program screen, this example and a few others below are shown with square brackets and sub-x for a polymer, whereas most examples in this paper are shown with conventional curved parentheses and a sub-x.

In the preceding 10 sections, 10 different types have been described, but there are potentially more categories than 10 because of the possibility that star polymers can be "mixed" types; for example, for star polymers that have more than one type of arm, some arms may be linear and others may be branched; similarly, some arms may be "homo", and others may be "ran./stat." or "block". These mixed types will not be described in this paper; the rules for indexing and naming them follow the general concepts illustrated for categories A-1 through A-10. These remarks apply also to the category B star polymers in the next section.

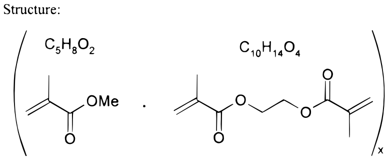
4.4. Category B Star Polymers. In category B, the star polymer center or core is itself polymeric (see point 2). The precise size and shape of the core and the number of arms emanating from it may be known, as is frequently the case with dendritic cores, or unknown, as is usually the case with hyperbranched cores. For polymers with hyperbranched cores, if the number of arms is known, it may be through post-synthetic analysis, rather than macromolecular design.

Point 2. For star polymers in categories B-1 through B-10, if the number of monomeric units comprising the core is known to be >10, the core is treated as a polymer; this is in accordance with CAS's rules for the indexing of polymers.[29] If the number of units is unknown or expressed as a fraction rather than an integer, the core is also treated as a polymer. If the number of units comprising the core is an integer <11, the core is treated as a discrete entity, and the polymer then belongs in category A. There is further discussion of this later in point 3.

Category B-1. All linear arms are identical (see note b under Table 1); each contains only one type of monomer unit or SRU. The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.1. Star polymer from methyl methacrylate and ethylene dimethacrylate (no nucleus; peripheral end group unknown).

Special input text descriptor: 8:DP,STA
Structure:

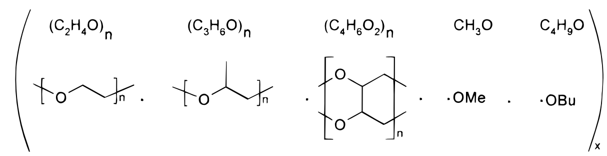


Polymer name: POLY-2-PROPENOIC ACID, 2-METHYL-, 1,2-ETHANEDIYL ESTER/2-PROPENOIC ACID, 2-METHYL-, METHYL ESTER, STAR
Text descriptors: POLY-HYPERCONNECTABLE; POLY-STAR

Category B-2. All linear arms are identical (see note b under table 1); each contains at least two types of monomer unit or SRU copolymerized in a random or statistical manner. The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.2. Star polymer from 1-butanol, methanol, methyloxirane, oxirane, and 1,2:3,4-diepoxybutane; methyloxirane and oxirane are polymerized simultaneously, and core formation is accomplished by subsequent addition of 1,2:3,4-diepoxybutane (no nucleus; peripheral end groups known).

Special input text descriptor: 8:DP,STA
Structure:

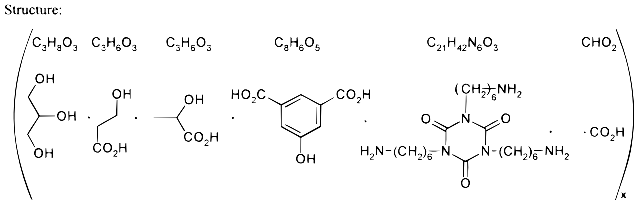


Polymer name: POLY-1,2,3,4-BUTANETETRAYL-2,3-BIS(OXY)/OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), STAR, END GROUP BUTOXY/METHOXY
Text descriptors: POLY-HYPERCONNECTABLE; POLY-STAR
Notes on example 4.4.2: (1) The 1,2,3,4-BUTANETETRAYL-2,3-BIS(OXY) component is hyperbranched, **not** a ladder segment. (2) The polymer is named ...END GROUP BUTOXY/METHOXY, rather than ...END GROUP BUTOXY, END GROUP METHOXY. The name style END GROUP BUTOXY/METHOXY indicates that any given peripheral end group is either a methoxy or a butoxy moiety.

Category B-3. All arms are identical (see note b under Table 1); each contains at least two types of monomer unit or SRU copolymerized in a random or statistical manner, and at least one monomer unit or SRU has a "connectivity" of more than two (i.e., it functions as a branching agent). The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.3. Star-branched polyester-urethane from glycerol (GL), hydracrylic acid (HA), 5-hydroxyisophthalic acid (5HI), "hexamethylene diisocyanate cyclic trimer" (HDCT), and lactic acid (LA): branched polyester arms formed from HA, LA, and 5HI; polyurethane microgel core formed from GL and HDCT (no nucleus; peripheral end groups known).

Special input text descriptor: 8:DP,STA
Structure:

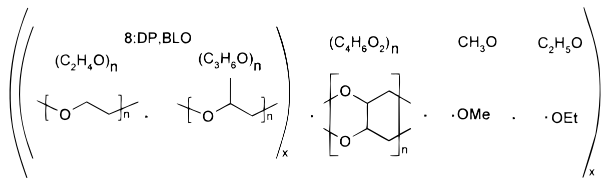


Polymer name: POLYESTER-URETHANE-1,3-BENZENEDICARBOXYLIC ACID, 5-HYDROXY-/1,2,3-PROPANETRIOL/PROPANOIC ACID, 2-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-/1,3,5-TRIAZINE-2,4,6(1H,3H,5H)TRIONE, 1,3,5-TRIS(6-AMINOHEXYL)-, STAR, END GROUP CARBOXY[30]
Text descriptors: POLYESTER-URETHANE; POLY-HYPERCONNECTABLE; POLY-STAR
Notes on example 4.4.3: (1) In common with all polymers in SCION (except for a few registered for special business purposes), no monomer unit or SRU ratios are cited; therefore the amount of 5HI is not part of the polymer record. (2) The information that the arms are polyester and the core is polyurethane is not stored; explanatory information may be added to the NOTES field if desired.

Category B-4. All linear arms are identical (see note b under Table 1); each contains at least two types of monomer unit or SRU copolymerized in a "blocky" manner. The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.4. Star polymer from ethanol, methanol, methyloxirane, oxirane, and 1,2:3,4-diepoxybutane; methyloxirane and oxirane are polymerized sequentially, and core formation is accomplished by subsequent addition of 1,2:3,4-diepoxybutane (no nucleus; peripheral end groups known).

Special input text descriptor: 8:DP,STA
Structure:

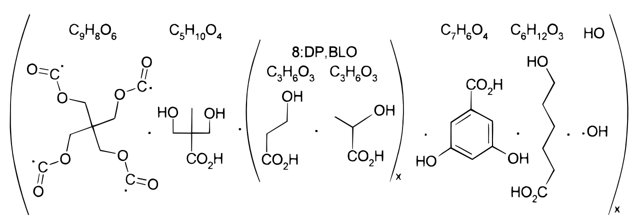


Polymer name: POLY-1,2,3,4-BUTANETETRAYL-2,3-BIS(OXY)/(OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), BLOCK), STAR, END GROUP ETHOXY/METHOXY
Text descriptors: POLY-BLOCK; POLY-HYPERCONNECTABLE; POLY-MULTILEVEL; POLY-STAR
Notes on example 4.4.4: (1) The 1,2,3,4-BUTANETETRAYL-2,3-BIS(OXY) component is hyperbranched, ***not*** a ladder segment, but CAS software limitations dictate its registration as a ladder polymer; (2) The polymer is named ...END GROUP ETHOXY/METHOXY, rather than ...END GROUP ETHOXY, END GROUP METHOXY. (3) The precise location of the "blocky" segment is indicated in this multilevel polymer. Multilevel polymer indexing has been discussed recently.[28] (4) The BLO block descriptor is applied at the poly-oxyethylene/oxypropylene level and is not applied also at the higher (star-polymer) level; however, the POLY-BLOCK descriptor is applied at the star-polymer level.

Category B-5. All arms are identical (see note b under Table 1); each contains at least two types of monomer unit or SRU copolymerized in a "blocky" manner, and at least one monomer unit or SRU has a "connectivity" of more than two (i.e., it functions as a branching agent). The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.5. Block star-branched polyester with a dendritic core (from a pentaerythritol nucleus and 2,2-bis-(hydroxymethyl)propionic acid), to which are attached branched polyester arms formed from caprolactone, 3,5-dihydroxybenzoic acid (branching monomer unit), and blocks of hydracrylic acid and lactic acid (nuclear and peripheral end groups known).

Special input text descriptor: 8:DP,STA
Structure:



Polymer name: POLYESTER-BENZOIC ACID, 3,5-DIHYDROXY-/HEXANOIC ACID, 6-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-2-(HYDROXYMETHYL)-2-METHYL-/(PROPANOIC ACID, 2-HYDROXY-/PROPANOIC ACID, 3-HYDROXY-, BLOCK), STAR, END GROUP HYDROXY, END GROUP OXY(CARBONYL)(1,3-PROPANEDIYL-2-YLIDENE-2-(METHYLENEOXYCARBONYL)-2-(METHYLENEOXYCARBONYL)-3-(OXYCARBONYL))

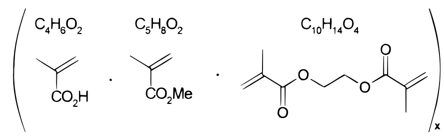
Text descriptors: POLY-BLOCK; POLYESTER; POLY-HYPERCONNECTABLE; POLY-MULTILEVEL; POLY-STAR

Notes on example 4.4.5: (1) In this example the arms contain blocks formed from hydracrylic acid and lactic acid. The structural representation contains no indication of: (a) how many generations are present in the dendritic core; (b) where the hydracrylic acid/lactic acid blocks and the 6-hydroxyhexanoic acid units (from caprolactam) are in the arms; (c) whether the hydracrylic acid/lactic acid blocks were preassembled or grown during synthesis of the complete star polymer; (d) where the 3,5-dihydroxybenzoic acid branching units are placed in the arms in relation to the 6-hydroxyhexanoic acid units and hydracrylic acid/lactic acid blocks. Were it necessary to distinguish between different structures, the special input text descriptor could be modified to assure uniqueness for each polymer, and explanatory information could also be added to the NOTES field. (2) This is another example of the CASRS's recently discussed capability of multiple-level polymer registration;[28] the hydracrylic acid/lactic acid block polymer carries an 8:DP,BLO designation, regardless of whether it is preassembled or not. The BLO designation is not repeated at the higher (star-polymer) level, but the POLY-BLOCK descriptor is applied at the star-polymer level.

Category B-6. Each arm *per se* is a linear homopolymer (see note b under Table 1); the composition of at least one arm differs from the others. The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.6. Separate "living polymerization" reaction mixtures of methacrylic acid and methyl methacrylate are physically combined, and the polymerization is continued with addition of ethylene dimethacrylate (no nucleus; peripheral end groups unknown).

Special input text descriptor: 8:DP,STA,VAR
Structure:

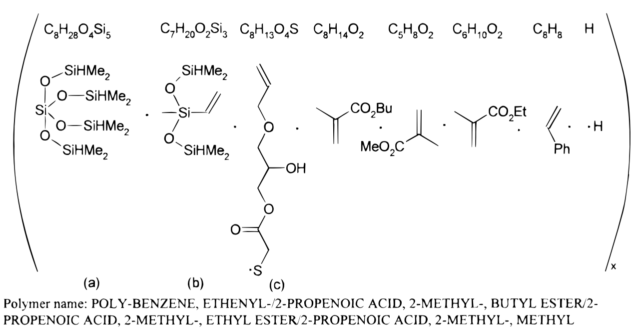


Polymer name: POLY-2-PROPENOIC ACID, 2-METHYL-/2-PROPENOIC ACID, 2-METHYL-, 1,2-ETHANEDIYL ESTER/2-PROPENOIC ACID, 2-METHYL-, METHYL ESTER, STAR
Text descriptors: POLY-HYPERCONNECTABLE; POLY-STAR; POLY-VARIEGATED

Category B-7. The composition of at least one arm differs from the others (see note b under Table 1); each arm *per se* is a linear polymer containing at least two types of monomer unit or SRU copolymerized in a random or statistical manner. The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.7.1. Star polymer with a dendritic core (from tetrakis(dimethylsiloxy)silane and 3-vinyl-1,1,3,5,5-pentamethyltrisiloxane), to which are attached two types of arms: a ran./stat. butyl methacrylate/methyl methacrylate copolymer and a ran./stat. ethyl methacrylate/styrene copolymer, both of which terminate in a (((3-(allyloxy)-2-hydroxypropoxy)carbonyl)methyl)thio end group[31] (nuclear fragment, bridging group, and peripheral end groups known).

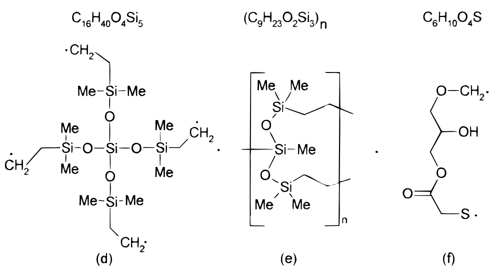
Special input text descriptor: 8:DP,STA,VAR
Structure:



Polymer name: POLY-BENZENE, ETHENYL-/2-PROPENOIC ACID, 2-METHYL-, BUTYL ESTER/2-PROPENOIC ACID, 2-METHYL-, ETHYL ESTER/2-PROPENOIC ACID, 2-METHYL-, METHYL ESTER/TRISILOXANE, 3-ETHENYL-1,1,3,5,5-PENTAMETHYL-, STAR, END GROUP HYDRO, END GROUP (((2-HYDROXY-3-(2-PROPENYLOXY)PROPOXY)CARBONYL)METHYL)THIO, END GROUP TRISILOXANE, 3,3-BIS((DIMETHYLSILYL)OXY)-1,1,5,5-TETRAMETHYL-
Text descriptors: END GROUP POLYMERIZABLE-CC; POLY-HYPERCONNECTABLE; POLY-STAR; POLY-VARIEGATED

Notes on example 4.4.7.1: (1) The dendritic core should ideally be represented by an SRU component, a "tetraradical" nucleus, and "diradical" bridging groups (see example 4.4.7.2); however, for reasons already discussed (see section 3.1), because it is not currently possible to register a three-crossing-bond SRU such as that shown in example 4.4.7.2, the dendritic part of the polymer is represented by the source-based structures shown as components (a) and (b). Component (c), which must now be represented as a monradical, represents the bridging groups formed by attachment of the arms to the core. (2) The nomenclature system used to derive this polymer name has been described elsewhere.[1] (3) From the presence of the POLY-VARIEGATED descriptor, it may be deduced that there is more than one arm type present; however, there is currently no indication of the precise composition of each type of arm. Such information could be added in the form of one or more text descriptors, or as a free-text explanation in the NOTES field. (4) Were it possible to represent the repeating unit of the core as a three-crossing-bond SRU, this star polymer would qualify for the POLY-MULTICATEGORY text descriptor;[1] because it is not, and all the repeat units are methacrylic or ethylenic, this descriptor is not used. (5) This example is close in concept to some work reported by Rubinsztajn[32] that involves reactions of $CH_2{=}CH\text{-}Si(\text{-}O\text{-}SiHMe_2)_3$ with acrylic copolymers H-[monomer unit(s)]$_x$-S-CH_2-O-CH_2-CH(OH)-CH_2-O-CH_2-CH$=$$CH_2$.

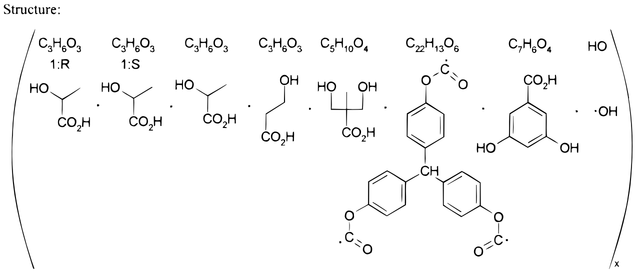
Example 4.4.7.2. Ideal, currently unregistrable SRU representation of the dendritic core of the polymer of example 4.4.7.1: (d) is the nucleus, (e) is the SRU, and (f) is the diradical bridging group.



Category B-8. The composition of at least one arm differs from the others (see note b under Table 1); each arm *per se* is a random (or statistical) copolymer. At least one branching monomer unit or SRU is also present, and at least one of the otherwise linear arms therefore contains branch points. The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.8. A branched star polyester with a dendritic core (from a 4,4′,4″-methylidynetris(phenol) nucleus and 3,5-bis(hydroxymethyl)benzoic acid), to which are attached two types of arms: (1) ran./stat. *R*-lactic acid/*S*-lactic acid, and (2) ran./stat. hydracrylic acid/lactic acid; each arm contains a small amount of 2,2-bis(hydroxymethyl)propionic acid as branching agent (nuclear and peripheral end groups known).

Special input text descriptor: 8:DP,STA,VAR
Structure:



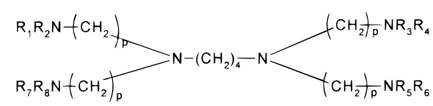
Polymer name: POLYESTER-BENZOIC ACID, 3,5-BIS(HYDROXYMETHYL)-/PROPANOIC ACID, 2-HYDROXY-/PROPANOIC ACID, 2-HYDROXY-, (R)-/PROPANOIC ACID, 2-HYDROXY-, (S)-/PROPANOIC ACID, 3-HYDROXY-/ PROPANOIC ACID, 3-HYDROXY-2-(HYDROXYMETHYL)-2-METHYL-, STAR, END GROUP HYDROXY, END GROUP METHYLIDYNETRIS(1,4-PHENYLENEOXYCARBONYL)
Text descriptors: POLYESTER; POLY-HYPERCONNECTABLE; POLY-STAR; POLY-VARIEGATED

Note on example 4.4.8: The symbols 1:R and 1:S are CAS stereo designations for *R* and *S* lactic acids, respectively.

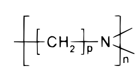
Category B-9. The composition of at least one arm differs from the others (see note b under Table 1); each arm *per se* is linear and "blocky". The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

Example 4.4.9 (see Chart 3). Star polymer (of structure already shown as example 3.1.2) with a dendritic[11] or hyperbranched[12] poly(1,3,5-benzenetriyl) core with >11 units (see point 3) converted to a variegated block-star polymer by condensation with a combination of nylon-66/nylon-6 blocks and nylon-6/nylon-11 blocks (nuclear and peripheral end groups known).

Point 3. De Brabander[33] cites preparation of star polymers from linear polymers (e.g., nylon-6), which become the star-polymer arms, and a dendritic core such as



wherein p is 1, 2, 3, etc. and R1 through R8 are -H, -$(CH_2)_3$-NH_2, -$(CH_2)_3$-N[$(CH_2)_3$-NH_2]$_2$, etc. Preparation of the star polymer of example 4.4.8 from the dendrimer or hyperbranched polymer of example 3.1.2 is an analogous case. In terms of indexing such a dendritic core in SCION, the number of occurrences of the SRU



(in the De Brabander case), or of the poly-3,3′,5,5′-biphenyltetrayl SRU (in the case of example 4.4.8) determines whether the core is treated as non-polymeric or polymeric.[29]

Category B-10. The composition of at least one arm differs from the others (see note b under Table 1); each contains at least two types of monomer unit or SRU copolymerized in a "blocky" manner, and at least one monomer unit or SRU has a "connectivity" of more than two (i.e., it functions as a branching agent). The core, which may contain a nonrepeating nucleus, is formed from at least one type of monomer unit or SRU that is capable of branching.

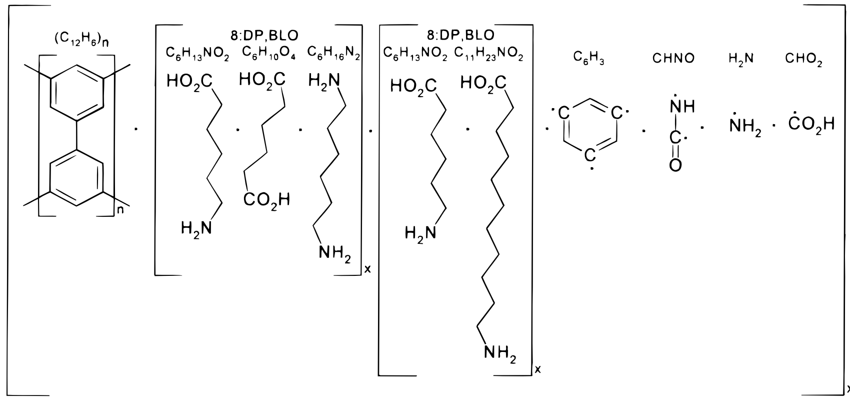
Example 4.4.10 (see Chart 4). A branched polyamide-ester star with two types of "blocky", branched arms: (1) from "MeO-(PEG/PPG, block)-NH_2" (e.g., Jeffamine* M-1000), caprolactam, and aspartic acid (branching agent); (2) from MeO-(PEG/PPG, block)-OH, caprolactone, and citric acid (branching agent). Both types of arm are end-capped with methacryloyl chloride, and the cross-linked acrylic core is from tetramethylene diacrylate.

5. THE FUTURE, AND SOME UNRESOLVED ISSUES

The dendrimer and star polymer field is still growing rapidly, and new structures are reported with increasing frequency. As more complex star polymers are developed, the current SCION rules will probably have to be extended, and perhaps new ones will have to be created, to keep pace with technological advances.

Chart 3

Special input text descriptor: 8:DP,STA,VAR
Structure:

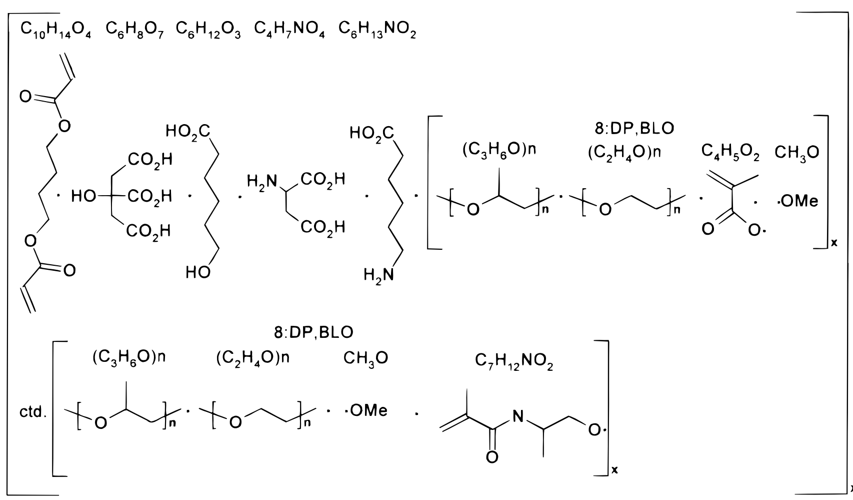


Polymer name: POLYAMIDE-(1,6-HEXANEDIAMINE/HEXANEDIOIC ACID/HEXANOIC ACID, 6-AMINO-, BLOCK)/(HEXANOIC ACID, 6-AMINO-/UNDECANOIC ACID, 11-AMINO-, BLOCK) WITH POLY-3,3′,5,5′-BIPHENYLTETRAYL, STAR, END GROUP 1,3,5-BENZENETRIYL, END GROUP AMINO/CARBOXY, END GROUP CARBONYLIMINO
Text descriptors: POLYAMIDE; POLY-BLOCK; POLY-HYPERCONNECTABLE; POLY-MULTILEVEL; POLY-STAR; POLY-VARIEGATED

[a] Notes on example 4.4.9: (1) From the presence of the POLY-VARIEGATED descriptor, it may be deduced that there is more than one arm type present, and it is known that there are nylon-66/nylon-6 and nylon-6/nylon-11 blocks; however, there is currently no indication of the precise composition of each type of arm. Should this become necessary, more precise special input text descriptors could be used to solve this problem. A free-text explanation in the NOTES field could also be added. (2) The carbonylimino "end group" indicates how the arms and core are joined; this star polymer has both carboxylic acid (-CO_2H) and amine (-NH_2) peripheral end groups because of the nylon-66/nylon-6 blocks; the nylon-6/nylon-11 blocks, of course, have only peripheral carboxy groups.

Chart 4

Special input text descriptor: 8:DP,STA,VAR
Structure:

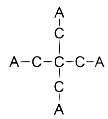


Polymer name: POLYAMIDE-ESTER-BUTANEDIOIC ACID, 2-AMINO-/HEXANOIC ACID, 6-AMINO-/HEXANOIC ACID, 6-HYDROXY-/(POLY-OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), BLOCK, END GROUP METHOXY, END GROUP 2-((2-METHYL-1-OXO-2-PROPENYL)AMINO)PROPOXY)/(POLY-OXY-1,2-ETHANEDIYL/OXY(1-METHYL-1,2-ETHANEDIYL), BLOCK, END GROUP METHOXY, END GROUP (2-METHYL-1-OXO-2-PROPENYL)OXY)/1,2,3-PROPANETRICARBOXYLIC ACID, 2-HYDROXY-, STAR
Text descriptors: END GROUP POLYMERIZABLE-CC; POLYAMIDE-ESTER; POLY-BLOCK; POLY-HYPERCONNECTABLE; POLY-STAR; POLY-VARIEGATED

[a] Notes on example 4.4.10: (1) This is another example of the CASRS multilevel indexing capability discussed in detail elsewhere.[28] (2) It is not possible to determine, from either the name or the structure, that some arms are polyamide and others are polyester; if both arms were polyamide-esters, the name and structure would be the same. If all arms were identical with regard to monomer unit content, the POLY-VARIEGATED descriptor would be omitted. If necessary, further details may be added via use of unique special input text descriptors and/or additional explanations in the NOTES field.

As an example of this, two recent papers by Gitsov and Fréchet[34,35] cite a four-arm star polymer with pentaerythritol as the core; each arm comprises a linear poly(oxy-1,2-ethanediyl) arm, at the periphery of which is a classical Fréchet wedge whose structure was shown as example 3.1.3 (see example 5.1).

Example 5.1. Fréchet combined star/dendritic polymer

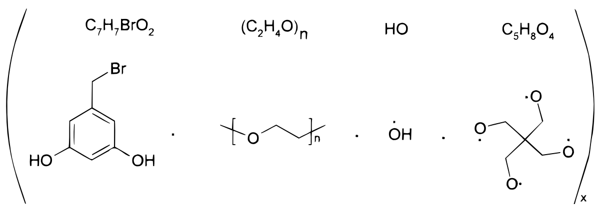


where A is -(O-CH_2-CH_2-)$_n$-O-W, and W is the Fréchet wedge shown as example 3.1.3.

The pending registration of this polymer in SCION poses a still-unresolved problem. The current SCION nomenclature rules result in the name and structure shown as example 5.2.

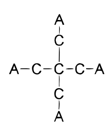
Example 5.2. SCION name and structure for Fréchet polymer of example 5.1.

Polymer name: POLY-1,3-BENZENEDIOL, 5-(BROMOMETHYL)- WITH POLY-OXY-1,2-ETHANEDIYL, END GROUP HYDROXY, END GROUP OXY-1,3-PROPANEDIYL-2-YLIDENE-2-(METHYLENEOXY)-2-(METHYLENEOXY)-3-OXY
Text descriptors: END GROUP, MULTICHAIN; POLY-HYPERCONNECTABLE; POLY-MULTICATEGORY
Structure:



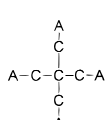
In addition to the confusion introduced by the need to use a source-based representation for the wedge SRU, which should ideally be represented by the structure of example 3.1.3, neither the name nor the structure enables a searcher to distinguish between the polymer described by Fréchet and other polymers with theoretical structures such as those shown as examples 5.3 and 5.4.

Example 5.3. Alternative theoretical structure derived from the components depicted and name given in example 5.2



where A is the Fréchet wedge; this implies a four-arm star polymer where each arm is a monodendron of structure shown as example 3.1.3. The periphery of each wedge is covered with hydroxy groups, to which can theoretically be attached linear poly(oxy-1,2-ethanediyl) arms.

Example 5.4. Alternative theoretical structure derived from the components depicted and name given in example 5.2



where A is a few SRUs (shown as example 3.1.3); to the peripheral OH groups are attached linear poly(oxy-1,2-ethanediyl) arms. These, in turn, are then attached to more wedge SRUs; and so on. This would comprise, overall, a branched star polymer with Fréchet monodendrons acting as branch points.

The structures of examples 5.1, 5.3, and 5.4 are all logical interpretations of the database record shown as example 5.2; steric reasons may prohibit the existence of the polymer depicted as example 5.3, but searchers may not know this and cannot be expected to deduce it from registration records.

This polymer closely resembles the one described as category A-5 and illustrated as example 4.3.5; neither that example nor this one is described uniquely, even by the combination of name and structure. Even in cases where explanations are added to the NOTES field, the complete record may not be entirely clear with regard to the complete polymer structure. This problem remains unresolved.

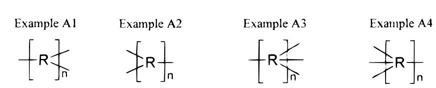
6. CONCLUSIONS

Classification and indexing methods have been described for dendritic and star polymers in DuPont's SCION proprietary database, and structure representations of 20 such polymers have been presented. Because this field of polymer science is still growing rapidly, new types will undoubtedly appear, and this paper must therefore be regarded as an initial attempt to deal with these types of polymers.

APPENDIX

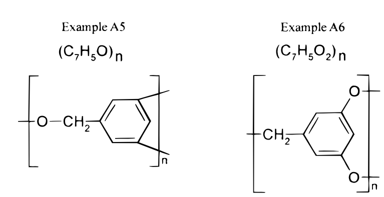
The SCION rules for defining, orienting, and naming SRUs were written before the need to register SRUs with unequal numbers of left- and right-crossing bonds such as A_3, AB_2, AB_3, etc. Registration of A_3-types is achieved by "doubling" them to A_4-types, as described in this paper. However, "doubling" fails for other types such as AB_2 and AB_3. The following additional rules were therefore written to cover these types. These two new rules precede the previously published rules 1 through 5,[19] which are now renumbered 3 through 7.

(New) Rule 1. The minimum number of crossing bonds of an SRU shall be on the left (i.e., pass thought the left-limiting parenthesis or bracket); the maximum number of crossing bonds of an SRU shall be on the right (i.e., pass thought the right-limiting parenthesis or bracket). Thus, in examples A1 through A4, in which R is any branching SRU, examples A1 and A3 are correct, whereas examples A2 and A4 are incorrect.



Note: If the numbers of left- and right-crossing bonds are equal, the SRU, whether it is single- or multiple-strand, is linear; ignore (new) rule 2 and proceed to rule 3 (old rule 1[16]).

(New) Rule 2. The branching moiety or subunit of the SRU shall be rightmost; this results in the minimum number of atoms needed to define the SRU. Thus, example A5 is correct, whereas example A6 is incorrect because the branching moiety is not rightmost and the MF contains one more oxygen atom.



ACKNOWLEDGMENT

The authors thank Dr. L. Wilczek of DuPont for sharing his technical knowledge and expertise on silane chemistry, and Mr. J. Donahue and Dr. D. Stauffer of MDL for acquisition of, and tutorials on, ISIS/Draw.

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(10) SCION polymer names begin POLY-... not POLY(... .[1]

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(17) Each SCION chemical-file record contains a free-text NOTES field that may be used, for example, for additional information not included in a polymer name or structure, which can help to elucidate the structure of a polymer.

(18) In a manner that parallels registration of a substance with a Registry Number in the CAS Registry File, a substance in SCION is registered with a CNUM (an acronym for C-Number). CNUMs cited in this paper are fictitious.

(19) Schultz, J. L.; Wilks, E. S. A nomenclature and Structural Representation System for Ladder and Spiro Polymers. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 786−796; Appendix.

(20) SCION nomenclature rules for AB_3-type SRUs are controlled by the same new rules (see *Appendix*) that control AB_2-type SRUs. In this case, phase-shifting to define an SRU with the minimum number of atoms results in the structure shown, in which oxygen is no longer the head atom.

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(22) Special input text descriptors are used primarily to prevent rejection by the CASRS of a polymer that has a different name and intellectual structure, but a structure identical with that of a previously registered polymer. Example: POLY-2-PROPENOIC ACID, 2-METHYL- vs. POLY-2-PROPENOIC ACID, 2-METHYL-, STAR. To avoid possible CASRS rejects, unnecessary registration delays and/or repeats, etc., it is customary to add routinely appropriate special input text descriptors such as the one shown; 8 denotes a CAS class 8 substance, DP is assigned by CAS to DuPont, and STA denotes a star polymer. CAS classifies polymers, radical ions, minerals, inorganic compounds, and incompletely defined structures as "class 8 substances".

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(26) "Blocky" arms in this context means "blocky" in the accepted sense of the word; thus, polymers containing backbones and/or arms of structure $-(M)_m-(M')_n-$ (where M and M′ are different SRUs or monomer units) [example (a)] are blocky. The question of what is or is not "blocky" is insufficiently defined in the polymer literature to cover all cases. The IUPAC definition of block,[24] "a portion of a macromolecule comprising many constitutional units, that has at least one feature which is not present in the adjacent portions", is precise enough to include polymers such as example (a). However, is not clear whether IUPAC's use of the word "feature" covers solely composition of monomer units or SRUs, or whether it also includes how many monomer units or SRUs are present. Thus, it is insufficiently explicit to indicate whether it includes polymers such as $-(M)_m-J-(M)_n-$ [(example (b)], in which different degrees of polymerization are present on each side of J (a non-repeating junction unit). IUPAC needs to modify its definition to include this point. CAS[29] does not address this point. By SCION rules, example (a) is considered to be a block polymer, whereas example (b) is not.

(27) Wang, L.; McKenna, S. T.; Faust, R. Initiation via Haloboration in Living Cationic Polymerization. 3. Synthesis and Characterization of Functional Star-Branched Polyisobutylenes. *Macromolecules* **1995**, *28*, 4681−4685; Tian, D.; Dubois, Ph.; Jerome, R.; Teyssie, Ph. Macromolecular Engineering of Polylactones and Polylactides. 18. Synthesis of Star-Branched Aliphatic Polyesters Bearing Various Functional End Groups. *Macromolecules* **1994**, *27*, 4134−4144; Simms, J. A. Recent Advances in the Use of Star Polymers in Coatings. *Progr. Org. Coat.* **1993**, *22*, 367−377.

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(29) Chemical Abstracts Index Guide, Chemical Abstracts Service, Columbus, OH, 1994, Appendix IV, Section 222.

(30) In SCION, polyurethanes are indexed not as multiisocyanates and multiols, but as multiamines (the corresponding theoretical parent of multiisocyanates) and multiols; the third theoretical parent in all polyurethanes, carbonic acid, is neither cited in the polymer name nor registered as a component of polyurethanes.[1] The prefix "multi" is used here to avoid any "polymeric" connotation.

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CI9700900