Orientation and Nomenclature of Multiple Radicals in Comb, Star, and Other Polymers with Multichain End Groups

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Received October 26, 1995⊗

Comb polymers with structural repeating unit (SRU) backbones, star polymers with discrete centers, and discontinuous linear polymers (i.e., polymers containing "spacer units") contain nonpolymeric moieties, called multiple radicals or multiradicals, that join the polymeric sequences. Computer-stored structures of these types of polymers in SCION, a DuPont proprietary chemical database, now include multiradicals as part of polymer structure records, and they are fully searchable polymer components. Rules for their orientation and nomenclature are presented.

1. INTRODUCTION AND BACKGROUND

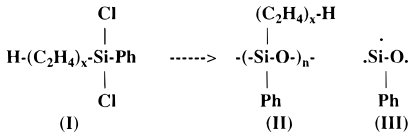
A recently published paper[1] discussed the indexing of comb polymers in SCION, a DuPont proprietary chemical database that uses Chemical Abstracts Service (CAS) STN MESSENGER software and is maintained for DuPont by CAS. Some comb polymers, especially those with backbones that are of the structural repeating unit (SRU) type (see Point 1), contain as part of their structure one or more moieties that join polymeric segments. In SCION these moieties may be either "repeating or "nonrepeating"; both types are called multiple radical or multiradical fragments. Example 1 shows a "repeating" moiety in a polymer.

Point 1: The International Union of Pure and Applied Chemistry (IUPAC) prefers the term "constitutional repeating unit" (CRU); the two terms are virtually synonymous.

Example 1. The polymer of structure I is hydrolytically polymerized to give the comb polymer of structure II (see Point 2).

Point 2: SCION polymer examples given are theoretical and may or may not have been reduced to practice.

The "repeating" moiety of the final polymer of structure II is the multiradical fragment III.



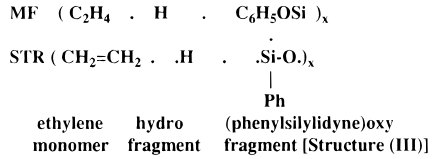
Polymer (I) name: POLY-ETHYLENE, END GROUP (DICHLOROPHENYLSILYL), END GROUP HYDRO (see Point 3).

Polymer (II) name: POLY-(POLY-ETHYLENE, END GROUP HYDRO, END GROUP (PHENYLSILYLIDYNE)-OXY) (see Point 4).

Point 3: By SCION nomenclature rules,[1] noncondensation type polymer names begin "poly-...", not "poly(..."; end groups are named "end group...", not ".alpha. ..." and ".omega. ...".

Point 4: In SCION, multiple parentheses are used in place of a combination of parentheses and square brackets; see convention 3 in section 2 below.

Polymer (II) is computer-stored as multicomponent structure IV (MF = molecular formula; STR = computer-stored structure):

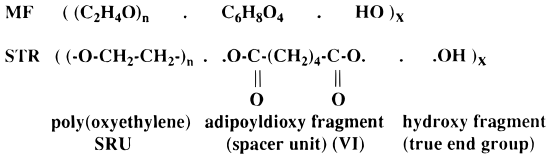


(IV)

An example of a "nonrepeating" moiety is a nonpolymeric "spacer unit" that joins two or more polymeric segments. The spacer unit in SCION corresponds to the "linking unit"[3] or "junction unit"[5] of the International Union of Pure and Applied Chemistry (IUPAC).

For multichain polymers other than comb types, spacer units are part of the computer-stored structure in the SCION database. Spacer units are represented structurally by multiradical fragments. Example 2 shows a "nonrepeating" moiety in a polymer.

Example 2. The polymer "HO-poly(oxyethylene)-(adipoyldioxy)-poly(oxyethylene)-OH" (V) contains the nonrepeating multiradical fragment (VI).



(V)

Polymer name: POLY-OXYETHYLENE, END GROUP ADIPOYLDIOXY, END GROUP HYDROXY (see Point 5).

Point 5. Reasons for calling the central multiradical fragment "adipoyldioxy" and not "adipoyl", and both end groups "hydroxy", are too complex to be discussed in toto here. The key point is to avoid splitting functional groups. The complete rationale is presented elsewhere.[1]

The phrase END GROUP in SCION polymer names is used both for true end groups that are on the ends of a polymer and for pseudo end groups that are multiradical fragments within a polymer. This simplifies polymer nomenclature by elimination of an additional phrase such as "spacer unit", "junction unit", "multiradical fragment", etc. The likelihood of confusion is minimal because mul-

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⊗ Abstract published in *Advance ACS Abstracts,* January 15, 1996.

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Table 1. Examples of Unitary Multiradicals

STRUCTURE	NAME	STRUCTURE	NAME
.O-O.	DIOXY	PH-PH	DIPHOSPHINEDIYL
:P-P:	DIPHOSPHINETETRAYL	SiH_2-SiH_2	DISILANYLENE
:SiH-O-SiH	DISILOXANEDIYLIDENE	.S-S.	DITHIO
:N-Me	(METHYLIMINO)	O=C-C=O	OXALYL
.O.	OXY	CH_2-C-CH_2	TRIMETHYLENE
.S-S-S.	TRITHIO	NH-C-NH ‖ O	UREYLENE

tiradical fragment names are sufficiently different from monoradical fragment names; compare "end group acetyl", "end group oxalyl", and "end group citroyl".

Multiradical fragments also form the center of some star polymers. In SCION, a polymer must have a multiradical fragment "connectivity" of at least three for it to be classified as a star polymer; thus V is not classified as a star polymer.

A multiradical fragment can also occur when, for example, a −CN or −CNO terminated polymer trimerizes to give a s-triazine ring.

As shown in structures IV and V above, registration of polymers in SCION includes end groups and multiradical fragments as components, and they are fully searchable as discrete chemical entities. Thus, in structure V, the adipoyldioxy fragment VI has a registration number, and it is searchable by name, structure, or molecular formula. Registration of polymers, including the avoidance of confusing fragments with free radicals, is described elsewhere.[1]

In contrast, in the CAS Registry file there is no registration of such individual fragments in the same way that (co)monomers or SRU components are registered. However, end groups and multiradical fragments do appear as part of the polymer name and also as a cumulative molecular expression outside the parentheses that denote the polymer. For example in structure VII, which shows the text-type terminal display for "polyethylene glycol with hydroxy end groups", the atoms comprising both end groups are added and expressed in the MF field as "H2 O"; the hydro (.H) and hydroxy (.OH) fragments are neither registered nor searchable as chemical entities.

RN 25322-68-3 LREGISTRY
CN Poly(oxy-1,2-ethanediyl), .alpha.-hydro-.omega.-hydroxy- (9CI) (CA INDEX NAME)
$
MF (C2 H4 O)n H2 O
$
STR H-(-O-CH_2-CH_2-)$_n$-OH

(VII)

Note: the $ symbol in structure VII indicates removal from the complete CAS display of text irrelevant to the discussion. The STR line is neatened for presentation here. The rest of the display is shown **exactly** as it appears online; e.g.; (C2 H4 O)n, not $(C_2H_4O)_n$, etc.

This paper presents a logical method for orienting and naming the multiple radicals in comb, star, and other polymers with multichain end groups.

2. CONVENTIONS AND SYMBOLS

Radical terms cited in this paper are defined as follows:

- monoradical: a fragment with one unpaired electron
- diradical: a fragment with two unpaired electrons
- triradical: a fragment with three unpaired electrons
- tetraradical: a fragment with four unpaired electrons (etc.)
- multiple radical or multiradical: a fragment with more than one unpaired electron

In this paper, three conventions are adopted:

1. In some structures the colon represents two electrons. The proximity of the two dots is NOT to be taken as indicating a pair of electrons; the colon is used as a way of showing two separate, single electrons on the same atom.
2. In accordance with CAS conventions for drawing structures, carbon atoms carrying unpaired electrons have ALL connecting atoms shown, including hydrogen atoms. Carbon atoms not carrying unpaired electrons need not have hydrogen atoms shown. For example, ".CH_2-" is shown with an unpaired electron and two hydrogen atoms, whereas "-C-" with no unpaired electrons means "-CH_2-" within a larger moiety.
3. Compound chemical names traditionally employing parentheses and brackets are represented by multiple parentheses, and brackets are eliminated. Thus, [(SELENYLMETHYL)SILYLIDYNE] is written as ((SELENYLMETHYL)SILYLIDYNE).

The multiradicals discussed in this paper are of two basic types: those namable by CAS rules for multiradicals[4] and those not namable by CAS rules.

3. MULTIRADICALS NAMABLE BY CAS RULES

A multiradical is namable by CAS rules[4] if it meets the two following criteria:

1. The central moiety (a) is unipart, i.e., its name is unitary (not derived by joining two or more preexisting unitary names); it may, however, be substituted, e.g., (methylimino) or (b) is two- (but not three- or more) part and named by unambiguously joining the unitary names of its two unipart moieties.
2. Further moieties, if any (a) are all identical with one another and (b) occupy all free valencies of the central moiety.

Note 1: the central moiety in 1(a) need not be symmetrical.

Note 2: a central moiety formed by joining two or more identical diradicals such that it is named by prefixing DI, TRI, etc. to the name of the diradical is unipart for the purposes of 1(a).

A unitary central moiety of a multiradical flanked by further IDENTICAL moieties may be used as a center for naming the entire multiradical. However, a "multipart" (parenthesized) central moiety of a multiradical may NOT be used as a center for naming the entire multiradical, even when it is flanked by further identical moieties. "Multipart" means that the name of the moiety is not a unitary name but is instead formed by joining two or more preexisting unitary names. Table 1 gives some examples of unitary multiradicals.

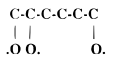
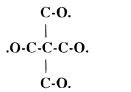
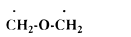
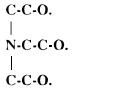
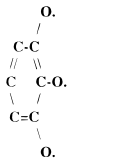
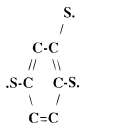
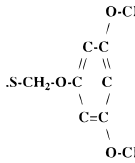
When a unitary multiradical is flanked by further identical moieties, the name begins with the unitary multiradical, continues with a prefix such as DI, BIS, TRI, TRIS, etc., and then states the rest of the multiradical. BIS (vice DI), TRIS (vice TRI), etc. are used when parentheses are required.

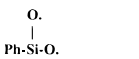
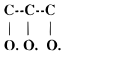
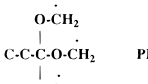
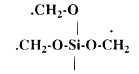
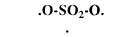
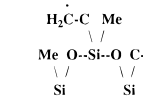
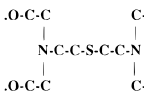
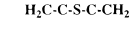
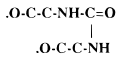
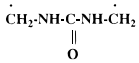
Examples of unitary diradicals flanked by identical moieties:

DIOXYDIMETHYLENE $\cdot CH_2$-O-O-$CH_2\cdot$

DIOXYBIS(ETHYLENETHIO) .S-C-C-O-O-C-C-S.

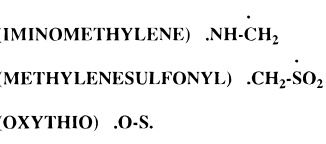
Table 2. Multiradicals with CAS Names or Namable by CAS Rules[a]

STRUCTURE	NAME
	1,2,6-HEXANETRIYLTRIOXY (Note 1)
	NEOPENTANETETRAYLTETRAOXY (Note 2)
	OXYBIS(ETHYLENEOXY)
	OXYDIMETHYLENE
	NITRILOTRIS (ETHYLENEOXY)
	v-PHENENYLTRIOXY
	as-PHENENYLTRITHIO
	s-PHENENYLTRIS (OXYMETHYLENETHIO)

STRUCTURE	NAME
	(PHENYLSILYLIDYNE)TRIOXY
	1,2,3-PROPANETRIYLTRIOXY
	PROPYLIDYNETRIS(OXYMETHYLENE)
	SILANETETRAYLTETRAKIS= (OXYMETHYLENE) (Note 5)
	SULFONYLDIOXY
	(2,4,6,8-TETRAMETHYLCYCLO= TETRASILOXANE-2,4,6,8-TETRA= YL)TETRAETHYLENE
	THIOBIS(ETHYLENENITRILO= BIS (ETHYLENEOXY)) (note 3)
	THIOBIS(ETHYLENEOXY)
	THIODIETHYLENE
	UREYLENEBIS(ETHYLENEOXY) (Note 4)
	UREYLENEDIMETHYLENE (Note 4)

[a] Note 1: The central moiety need not be symmetrical so long as it has a unitary name. Note 2: The largest starting unitary moiety possible must be selected; thus, METHANETETRAYLTETRAKIS(METHYLENEOXY) is incorrect. Note 3: A peripheral moiety may itself have further peripheral moieties. Note 4: Structurally, ureylene is multipart, but, as shown in Table 1, because it has a CAS unitary name, this name is acceptable. Note 5: Polymer or radical names that continue without a space on the next line are indicated by an "=" sign at the right-hand end of the line.

Examples of two-part multiradicals:



(IMINOMETHYLENE) .NH-CH_2.

(METHYLENESULFONYL) .CH_2-SO_2.

(OXYTHIO) .O-S.

The final names in these three examples are derived by alphabetization of the two unitary diradicals; thus, for the second one the "methylene + sulfonyl" name derivation in this system has no connection with CAS atom priority rules (S is senior to C).

CAS names two-part multiradicals only when they are not flanked by further moieties. When multipart multiradicals are flanked by further moieties, CAS does not name them by this method, even if the flanking moieties are identical. Thus, CAS does NOT use the name (METHYLENESULFONYL)DIOXY for the multipart multiradical ".O-CH_2-SO_2-O.". SCION rules are used to derive the name OXYMETHYLENESULFONYLOXY—see section 4.1 below. Table 2 shows selected multiradicals that either have CAS names or can be named according to CAS rules.

4. MULTIRADICALS NOT NAMABLE BY CAS RULES

For multiradicals not namable by CAS rules, SCION rules were developed; the rest of this section is devoted to explaining them.

4.1. Diradicals. As a logical extension of the CAS eighth Collective Index (8CI) rules for naming two-part, unsymmetrical, multiplying radicals (e.g., methylenesulfonyl, not sulfonylmethylene),[4a] SCION names for diradicals are "nomenclature-driven", not "structure-driven". The final name of a multipart diradical is derived by naming each unitary moiety in turn and proceeding through the entire multipart diradical from one end to the other. This process is hereby defined as the "walk-through naming method"; it is applicable only because there is only one starting point and one finishing point. In the "walk-through naming method", the first and last unitary moieties to be cited in the complete multipart diradical name must either (a) be or (b) contain an atom carrying an unpaired electron.

Example of (a): .CH_2--- METHYLENE...

Example of (b): .CH_2-C-C--- TRIMETHYLENE...

Depending upon which end is selected to begin the naming, two names result from this process; the one that alphabetizes first is selected. Starting in the middle and using DI, BIS, TRI, TRIS, etc., is forbidden.

Example 3: OXYMETHYLENESULFONYLOXY

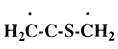
.O-SO_2-CH_2-O.

EXPLANATION OF NAME DERIVATION: naming this diradical from left to right gives OXYSULFONYLMETHYLENEOXY. Naming it from right to left gives OXYMETHYLENESULFONYLOXY; the latter alphabetizes before the former and is therefore the selected name. Starting in the middle and using the CAS rule of "treating like things alike" (see Point 6), with regard to the OXY moieties, is forbidden; thus (METHYLENESULFONYL)DIOXY is unacceptable because (METHYLENESULFONYL) is not a unitary name.

Point 6. This rule was superseded by the rule "You must multiply when you can". Neither rule is acceptable in SCION for naming diradicals because of the risks of ambiguity and confusion in nomenclature.

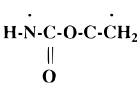
Further examples are given to illustrate the method.

Example 4: ETHYLENETHIOMETHYLENE

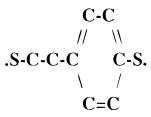


Example 5: OXYETHYLENETHIO

Example 6: ETHYLENEOXYCARBONYLIMINO



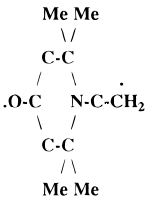
Example 7: THIOETHYLENE-P-PHENYLENETHIO



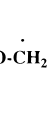
Note: both ends begin THIO; therefore, ETHYLENE and PHENYLENE are the moieties that determine the name, and ETHYLENE alphabetizes before PHENYLENE.

Side-chain substitution in moieties is handled by normal conventions—see examples 8−16.

Example 8: ETHYLENE(2,2,6,6-TETRAMETHYL-1,4-PIPERIDINEDIYL)OXY

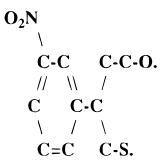


Example 9: METHYLENEOXY(METHYLPHENYLSILYLENE)OXY-P-PHENYLENE(METHYLIMINO)ETHYLENEOXY



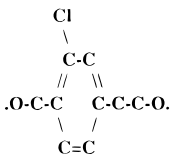
Example 10: (DIPHENYLSILYLENE)ETHYLENEOXY

Example 11: OXY(3-(M-NITROPHENYL)TETRAMETHYLENE)THIO



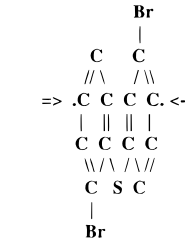
Substituents in a ring in the middle of a sequence of moieties that make up a diradical are numbered from where the ring is entered, as in the following example.

Example 12: OXYETHYLENE(3-CHLORO-P-PHENYLENE)METHYLENEOXY



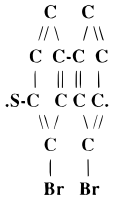
Note: the "walk-through naming method" gives OXYMETHYLENE(2-CHLORO-P-PHENYLENE)ETHYLENEOXY and OXYETHYLENE(3-CHLORO-P-PHENYLENE)METHYLENEOXY as the two possible names. OXYETHYLENE... alphabetizes before OXYMETHYLENE..., and the selected name, OXYETHYLENE(3-CHLORO-P-PHENYLENE)METHYLENEOXY, places the chloro group in the 3 position.

Example 13: (2-BROMO-P-PHENYLENE)THIO(2-BROMO-P-PHENYLENE)

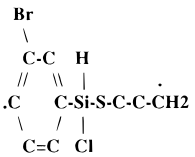


Note: naming starts at the single-shaft arrow; starting at the double-shaft arrow gives (3-BROMO-P-PHENYLENE)-THIO(3-BROMO-P-PHENYLENE), which violates the rule that, all other criteria being satisfied, lowest-possible locant numbers must be used.

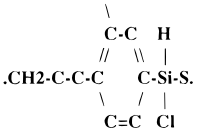
Example 14: (3,3'-DIBROMO-4,4'-BIPHENYLYLENE)THIO



Example 15: (2-BROMO-P-PHENYLENE)(CHLOROSILYLENE)THIOTRIMETHYLENE



Example 16: THIO(CHLOROSILYLENE)(3-BROMO-P-PHENYLENE)TRIMETHYLENE



4.2. Triradicals, Tetraradicals, Pentaradicals, Etc. For multiradicals carrying more than two unpaired electrons,

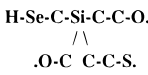
there is no simple way of naming them because the atom-by-atom path between the atoms carrying unpaired electrons is no longer unidirectional as it was for diradicals, and the "walk-through naming method" fails to cover all the possibilities. Therefore, new rules are needed to determine where to start and how to proceed.

Rule 1. A highest priority path-atom (HPPA) in the multiradical is selected, according to the SCION database chemical file atom priority rules (see Point 7).

Point 7: the full set of SCION database chemical file rules is given elsewhere.[2] The rule relevant here is as follows: The highest-priority atom is the one with the highest atomic number. Thus, the order is Bi, Pb, Hg, Te, Sb, Sn, Se, As, Ge, S, P, Si, O, N, B, etc. This contrasts sharply with CAS and IUPAC rules that rank atoms in the following order: O, S, Se, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Hg, etc.

Rule 2. The HPPA selected in Rule 1 must be in a "walk-through path". A "walk-through path" is any continuous path through the multiradical that begins with an atom carrying an unpaired electron and ends with an atom carrying an unpaired electron. Thus, in example 17, although Se is the heaviest atom in the multiradical, it is disqualified as the HPPA because it is not in any "walk-through path".

Example 17: THIOETHYLENE((SELENYLMETHYL)SILYLI=DYNE)(ETHYLENEOXY)(METHYLENEOXY)



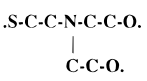
Rule 3. The HPPA—with, of course, any "dead-end" (nonpath) substituents—is cited in the name of the multiradical before any other path-atom; if the HPPA is in a ring or ring system, the ring or ring system containing the HPPA is named.

Rule 4. Each "moiety sequence" radiating outward from the HPPA is named. A "moiety sequence" is a sequence of moieties joined in a chain or string that ends in an atom with at least one unpaired electron.

Rule 5. If there is more than one moiety sequence, the sequence names are alphabetized. Moiety sequence names containing two or more unitary diradicals are parenthesized.

Rule 6. Moving along more than one path at a time within a multiradical is forbidden. When path branching occurs in a moiety sequence, each sequence, including unitary multiradical ones, that follows the atom or group at which branching occurs is parenthesized, and the sequence names are alphabetized. If two or more moiety sequences with identical names occur after branching, the name of each must be cited separately; use of DI, BIS, etc. is forbidden—see example 18.

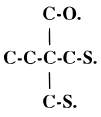
Example 18: THIOETHYLENENITRILO(ETHYLENEOXY)(ETH=YLENEOXY), not THIOETHYLENENITRILOBIS(ETHYLENEOXY)



Rule 7. The largest-possible moiety is always taken in preference to smaller moieties. Carbon chains may not be broken. See example 19 following Rule 8.

Rule 8. If there are two or more equally eligible HPPAs, e.g., in example 19, one is selected, the resulting moiety sequences are named, and the sequence names are alphabetized.

Example 19: THIO-1-BUTANYL-2-YLIDENE(2-(METHYLENE=OXY))(2-(METHYLENETHIO))



Note 1: Pedantically, the name should be 1-THIO-1-BUTANYL-... , but attachment of the THIO moiety to the 1- position can be deduced because locants of all other substituents are stated explicitly; it is, therefore, unnecessary to cite the 1-.

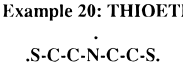
Note 2: The name BIS(THIOMETHYLENE)-1-BUTANYL-2-YLIDENE-1-OXY is unacceptable, because it is derived by simultaneous application of the "walk-through naming method" to two different paths—a violation of Rule 6.

Note 3: A name such as (THIOMETHYLENE)PROPYLIDYNE(METHYLENEOXY)(METHYLENETHIO) is unacceptable because it breaks a four-carbon chain—a violation of Rule 7.

The CAS rules of "treat like things alike" and "you must multiply when you can" are ignored, because it is either impossible or too confusing to apply the "walkthrough naming method" to more than one moiety sequence at a time.

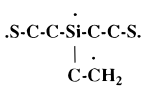
Further examples illustrate the method.

Example 20: THIOETHYLENENITRILO(ETHYLENETHIO)

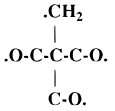


Sometimes, as in example 20, moieties appear to have been inadvertently omitted, but this indicates a multiradical, e.g., NITRILO, that has an unpaired electron and also groups. Because NITRILO is a branch point, the rest of the moiety sequence is parenthesized per Rule 6, even though only one moiety sequence is attached. See also the two following examples.

Example 21: THIOETHYLENESILANETETRAYL(ETHYLENE)=(ETHYLENETHIO)

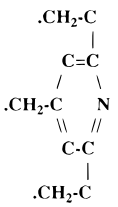


Example 22: OXYNEOPENTANETETRAYL(OXY)(OXY)



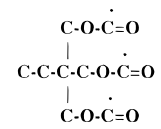
Note: The name OXYNEOPENTANETETRAYLDIOXY is incorrect for two reasons: (1) the DIOXY diradical is .O-O. and (2) such a name implies simultaneous application of the "walk-through naming method" to two different paths—a violation of Rule 6.

Example 23: 2,4,6-PYRIDINETRIYL-2-ETHYLENE-6-ETHYLENE-=4-METHYLENE



Note: this example illustrates application of Rule 3.

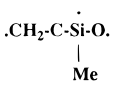
Example 24: OXY(1-BUTANYL-2-YLIDENE(2-(METHYLENEOXY=CARBONYL))(2-(METHYLENEOXYCARBONYL)))CARBONYL



Note: This example illustrates the nomenclature method for situations where the head atom is not at an end of the multiradical; the moieties emanating from the head atom are named and then alphabetized in the final multiradical name. Where necessary, parentheses are used for clarification.

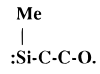
Example 25: (METHYLSILYLIDYNE)OXY

Example 26: (METHYLSILYLIDYNE)ETHYLENEOXY

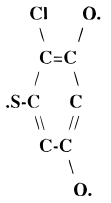


Compare the name for example 26, in which the omission of parentheses indicates that ETHYLENE and OXY are two separate unitary multiradicals joined to the HPPA (METHYLSILYLIDYNE), with the next example, in which ETHYLENE and OXY are parenthesized as (ETHYLENEOXY) to indicate that the two moieties are connected in a linear "string".

Example 27: (METHYLSILYLIDYNE)(ETHYLENEOXY)

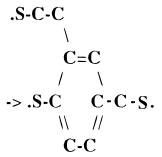


Example 28: THIO-(2-CHLORO-s-PHENENYL)(OXY)(OXY)



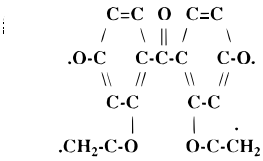
Note: Pedantically, the name should be THIO-(2-CHLORO-s-PHENENYL)(3-OXY)(5-OXY); however, by deduction, the OXY moieties can only be at the 3- and 5-positions. Had the sulfur atom been para to the chlorine atom, the name would have been THIO-(4-CHLORO-s-PHENENYL)(OXY)(OXY). Therefore, it is unnecessary to state the positions of the OXY moieties in the name.

Example 29: THIO-as-PHENENYL(2-(ETHYLENETHIO))(4-(METHYLENETHIO))



Note: The sulfur with the arrow is selected as HPPA because it is in a more crowded/heavier environment than the other sulfur;[2] entry into the as-phenenyl (1,2,4-benzenetriyl) ring system is placed at the 1 position.

Example 30: OXY-as-PHENENYL(1-(CARBONYL-as-PHENENYL=(4-OXY)(2-OXYETHYLENE)))(2-(OXYETHYLENE))



5. SUMMARY

Rules for the orientation and nomenclature of multiple radicals (multiradicals) have been presented. Multiradicals are nonpolymeric moieties that join polymeric sequences in comb, star, and other polymers with multichain end groups. Multiradicals are included as part of polymer structure records in SCION, a DuPont proprietary chemical structure database, and they are fully searchable as polymer components.

REFERENCES AND NOTES

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(2) Schultz, J. L.; Wilks, E. S. A Nomenclature and Structural Representation System for Ladder and Spiro Polymers; Appendix (SCION Database Chemical File: Atom Priority Rules). Submitted for publication.

(3) International Union of Pure and Applied Chemistry. Structure-Based Nomenclature for Irregular Single-Strand Organic Polymers. *Pure Appl. Chem.* **1994**, *66*(4), 873−889.

(4) Chemical Abstracts Service (Copyright 1969, the American Chemical Society). Naming and Indexing of Chemical Compounds (1969 ed): (a) Sections 117−120 (pp 375−390).

(5) Bareiss, R. E.; Kahovec, J.; Kratochvil, P. Graphic Representations (Chemical Formulae) of Macromolecules (International Union of Pure and Applied Chemistry). *Pure Appl. Chem.* **1994**, *66*(12), 2469−2482.

CI950163K