

STN[®]

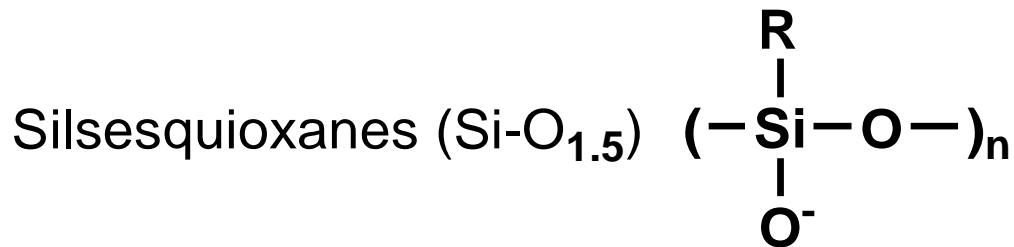
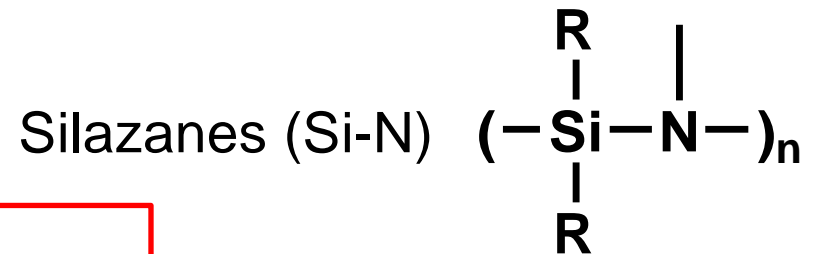
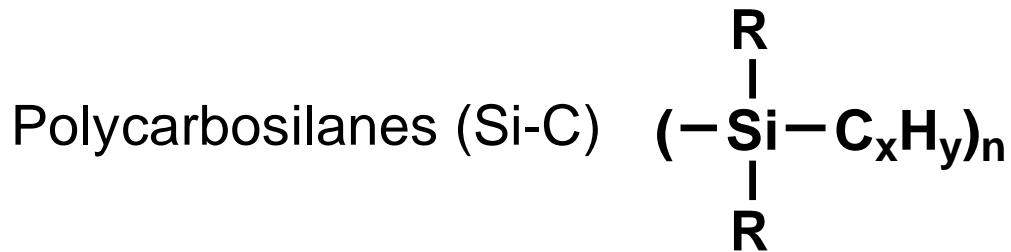
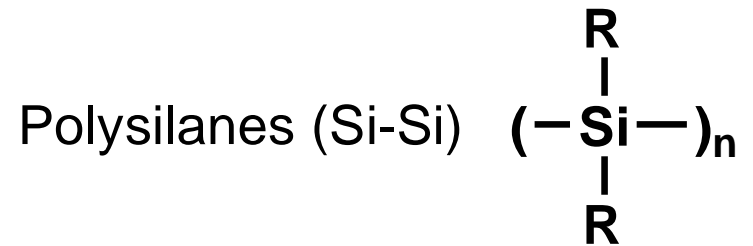
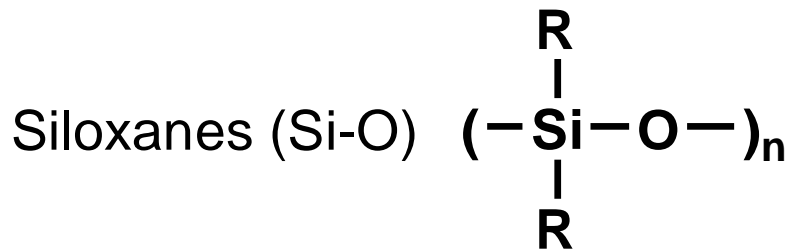
Searching for silicone (polysiloxane)
information on STN[®]

Robert Austin – FIZ Karlsruhe

Agenda

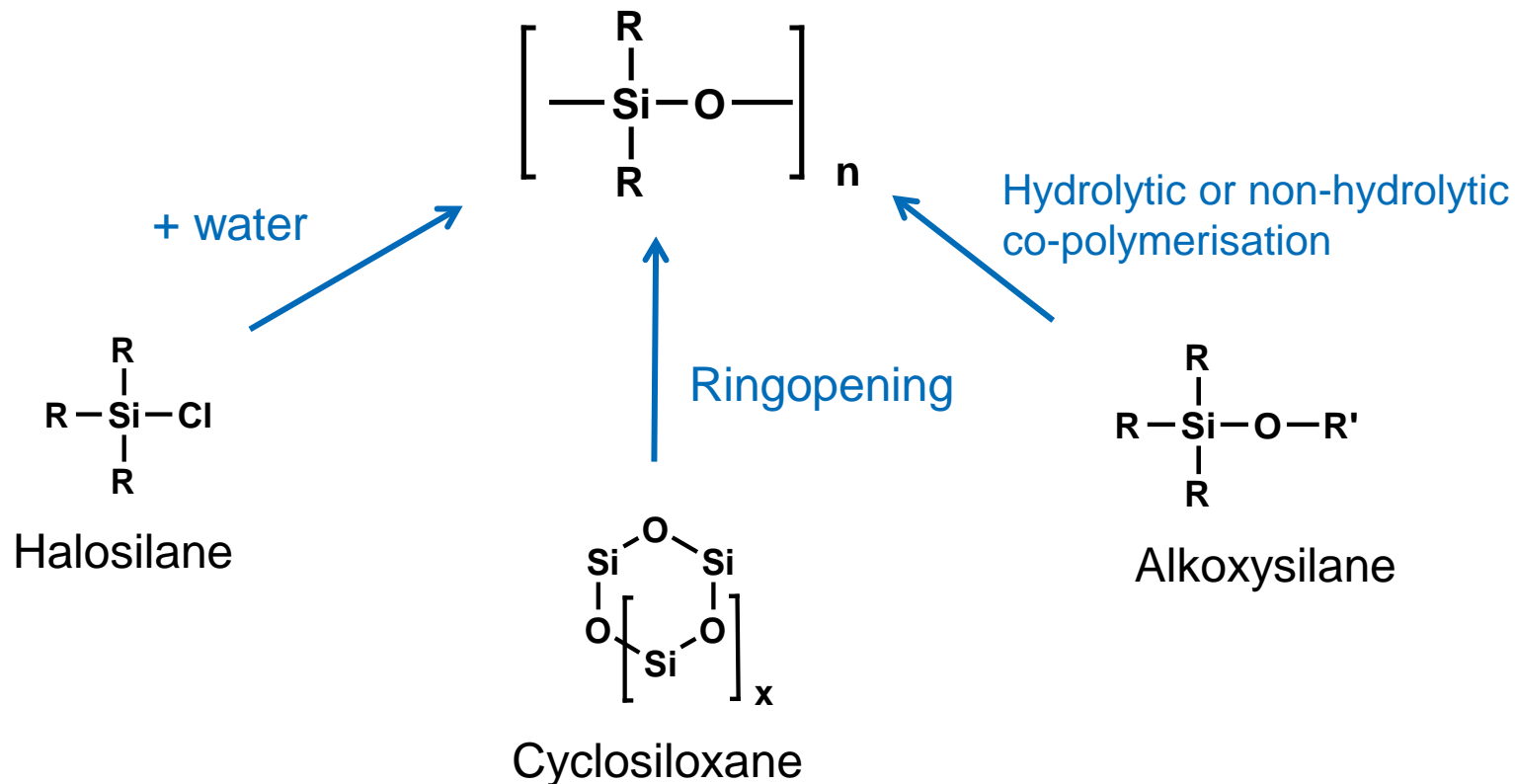
- Types of silicon polymers
- Polysiloxanes in CAplus/REGISTRY
 - Alkoxysilane-based polysiloxanes
 - Halosilane-based polysiloxanes
 - Polysiloxanes prepared by ring-opening polymerization
 - Single-unit polysiloxane SRUs
 - Multi-unit polysiloxane SRUs
 - Silsesquioxanes
- Polysiloxanes in DWPI Polymer Indexing
- Polysiloxanes in DWPI Chemistry Resource (DCR)

Types of silicon polymers



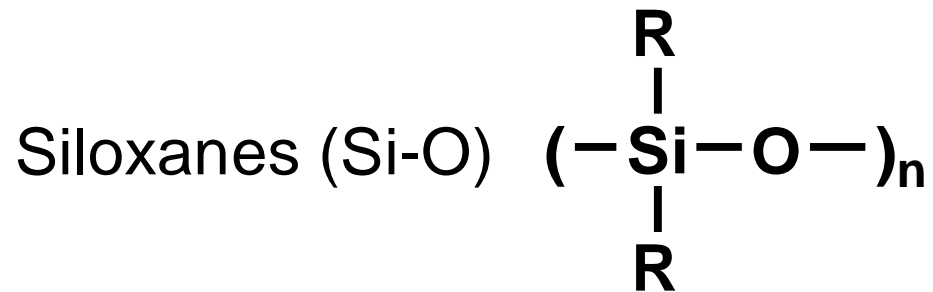
Polysiloxanes

Syntheses of Polysiloxanes



Note: It is important to be aware of the synthetic pathways as it helps understand database indexing.

Polysiloxanes in CPlus



- Controlled terms:**
- Polysiloxanes** (1997-present)
 - Siloxanes and Silicones** (1972-1996)
 - Siloxanes** (1937-1971)
 - Silicones** (1937-1966)
 - Cyclosiloxanes** (1937-) (nonpolymeric)

Polysiloxanes in REGISTRY

1994- : All polysiloxanes receive a CAS RN (monomer based and/or SRU)

Before

1994: Polysiloxanes prepared by *non-hydrolytic* methods received CAS RN

PCT: Polyother or manual registration

Unspecified (approx. 1900 substances):
CN: "Siloxanes and Silicones"
PCT: Manual registration

CAS indexing before 1994

Siloxane polymers prepared by **hydrolytic condensation** of chlorosilanes or alkoxy silanes did not receive CAS RNs for the polymer prior to June 1994. For example, the polysiloxane prepared from hydrolytic polymerization of dichlorodimethylsilane had no CAS RN indexing for the polymer, but would be indexed with the heading “Siloxanes and Silicones”, or Siloxanes.

```
IT      Siloxanes and Silicones, uses  
        (di-Me, potting with, electronic devises)
```

A monomer based entry was made if there were reaction studies or preparative studies:

```
IT      75-54-7, dichlorodimethylsilane  
        (hydrolytic polymn of,.....)
```

Polysiloxane types

1. Alkoxysilane-based polysiloxanes
2. Halosilane-based polysiloxanes
3. Single-unit polysiloxanes SRUs
4. Multi-unit polysiloxanes SRUs
5. Siloxane components in copolymers
6. Silsesquioxanes

Polysiloxanes in REGISTRY

Alkoxysilane-based polysiloxanes (hydrolytic polymerization or copolymerization of alkoxysilanes) (1994-)

Registry: Monomer based indexing +
SRU (only for single unit type)

Halosilane-based polysiloxanes (hydrolytic polymerization) (1994-)

Water is included in the polymer registration and is incorporated in the polymer name, but is not handled as a monomer in the name.

Registry: -Monomer based indexing + “hydrolytic”;
Water appears as separate component
+
- SRU (only for single unit type)

Alkoxysilane-based polysiloxanes

A polysiloxane from hydrolytic polymerization of Me₂Si(OMe)₂

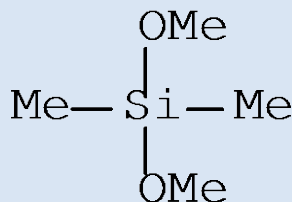
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2013 ACS on STN
RN **25498-04-8** REGISTRY
CN Silane, dimethoxydimethyl-, homopolymer (CA INDEX NAME)
MF (C4 H12 O2 Si)_x
CI PMS
PCT Polyether, Polyether only

****RELATED POLYMERS AVAILABLE WITH POLYLINK**** ←

CM 1

CRN 1112-39-6

CMF C4 H12 O2 si



SRU is RN 9016-00-6: Poly[oxy(dimethylsilylene)].

Halosilane-based polysiloxanes

A polysiloxane from hydrolytic polymerization of Me₂SiCl₂

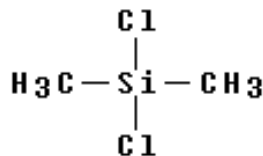
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2013 ACS on STN
RN 158158-00-0 REGISTRY
CN Silane, dichlorodimethyl-, homopolymer, hydrolytic
MF (C2 H6 Cl2 Si . H2 O)_x
CI PMS, COM
PCT Polyother, Polyother only

****RELATED POLYMERS AVAILABLE WITH POLYLINK****

CM 1
CRN 7732-18-5
CMF H2 O

H₂O

CM 2
CRN 75-78-5
CMF C2 H6 Cl2 si



SRU is RN 9016-00-6: Poly[oxy(dimethylsilylene)].

Polysiloxanes in REGISTRY

Polysiloxanes prepared by **ring-opening** polymerization of cyclosiloxanes (1907-)

Registry: Monomer based indexing of the cyclosiloxane + SRU (only for single unit type)

Single-unit polysiloxanes

Registry: SRU + Monomer based indexing assuming hydroxysilanes for the monomers.

Polysiloxanes prepared by ring-opening polymerization

Homopolymer of octamethylcyclotetrasiloxane

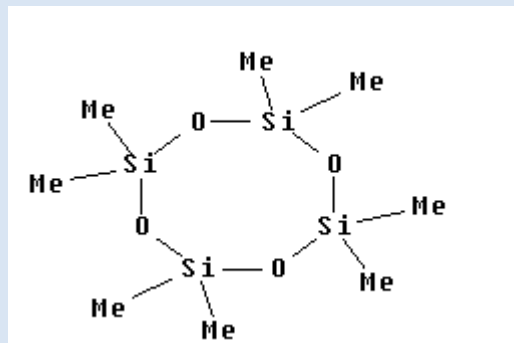
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2013 ACS on STN
RN 25037-57-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-, homopolymer
(CA INDEX NAME)

****RELATED POLYMERS AVAILABLE WITH POLYLINK****

CM 1

CRN 556-67-2

CMF C8 H24 O4 Si4



SRU is RN 9016-00-6: Poly[oxy(dimethylsilylene)].

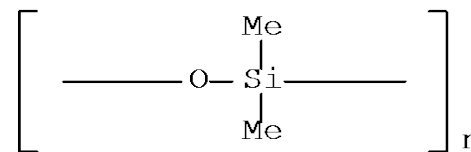
Single-unit polysiloxane SRUs

Example:

A polysiloxane with the author representation of (-OSiMe₂-)_n or "poly(dimethylsiloxane)" with no preparative information and no end groups specified.

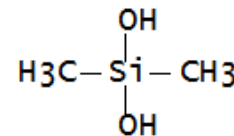
Indexed with an SRU

RN 9016-00-6: Poly[oxy(dimethylsilylene)]



In addition, a monomer-based polymer is indexed with the relevant hydroxysilane as an *assumed monomer*

RN 31900-57-9: Silanediol, dimethyl-, homopolymer



Single-unit polysiloxane SRUs (cont.)

Both the SRU-based RN and the assumed monomer based RN are indexed over in CPlus, e.g.:

CC 76-3 (Electric Phenomena)
Section cross-reference(s): 38, 39, 77

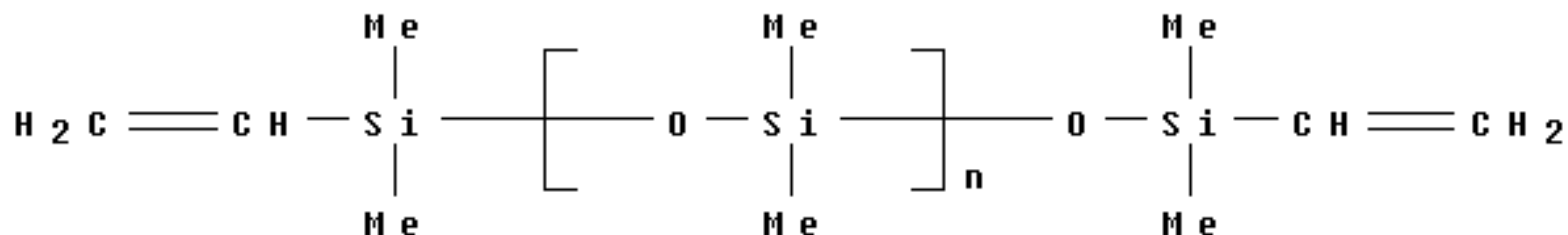
IT 31900-57-9, Polydimethylsiloxane
RL: PRP (Properties)
(assumed monomer, rubber, high temperature vulcanizing, protective sealant coating material; corrosion-resistant coating system for a dry-type transformer core)

IT 9016-00-6, Poly[oxy(dimethylsilylene)]
RL: PRP (Properties)
(rubber, high temperature vulcanizing, protective sealant coating material; corrosion-resistant coating system for a dry-type transformer core)

Single-unit polysiloxane SRUs with end groups

Example:

A polysiloxane with an author representation:



Indexed with the given SRU:

RN: **59942-04-0** MF: (C2 H6 O Si)_n C8 H18 O Si2

CN: Poly[oxy(dimethylsilylene)], **.alpha.**-(ethenyldimethylsilyl)-**.omega.**-[(ethenyldimethylsilyl)oxy]-

And/Or: Indexed with the **assumed** monomer (Me₂Si(OH)₂)_x with derivative "D", i.e. **31900-57-9D**, and terminating groups in the CPlus modifying phrase

Single-unit polysiloxane SRUs with end groups

The SRU-based RN and/or the assumed monomer based RN are indexed over in CPlus, e.g.:

CC 38-3 (Plastics Fabrication and Uses)
Section cross-reference(s): 39

IT 31900-57-9D, Dimethylsilanediol homopolymer, vinyl-terminated
RL: POF (Polymer in formulation); TEM (Technical or engineered material use); USES (Uses)
(assumed monomers, rubber; synthesis of silicone ionomer membranes and the use thereof)

IT 59942-04-0, Vinyl-terminated polydimethylsiloxane
RL: POF (Polymer in formulation); TEM (Technical or engineered material use); USES (Uses)
(rubber; synthesis of silicone ionomer membranes and the use thereof)

Multi-unit polysiloxane SRUs

Example:

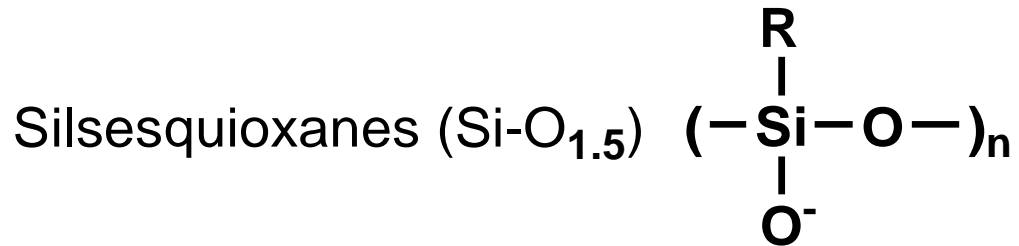
A polysiloxane represented by the author as $(-\text{OSiMe}_2)_x(-\text{OSiPh}_2)_y$ with no preparative information given.

No indexing with an SRU!

A monomer-based polymer entry is made by assuming hydroxysilanes for the monomers:

```
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2013 ACS on STN
RN 156048-34-9 REGISTRY
ED Entered STN: 30 Jun 1994
CN Silanediol, 1,1-dimethyl-, polymer with 1,1-diphenylsilanediol (CA
INDEX NAME)
MF (C12 H12 O2 Si . C2 H8 O2 Si)x
CI PMS, COM
PCT Polyother, Polyother only
```

Polysilsesquioxanes



In Registry: Monomer-based polymer (Hydroxysilane monomers are assumed) (1994-)

SRUs for the ladder type (1994-) when a single RSiO_{1.5} unit is given

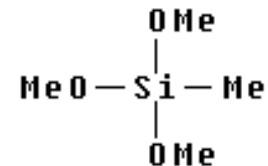
In CPlus:

Controlled terms: Silsesquioxanes (1947-)

Polysilsesquioxanes (cont.)

Example:

Polymethylsilsesquioxane from hydrolytic polymerization of methyltrimethoxysilane

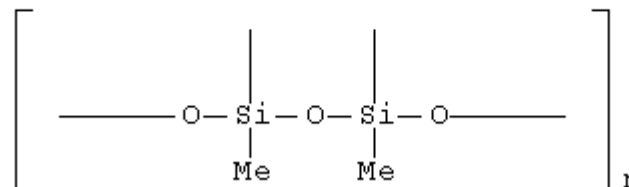


A monomer-based polymer entry is made:

```
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2013 ACS on STN
RN 25498-03-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN Silane, trimethoxymethyl-, homopolymer (CA INDEX NAME)
MF (C4 H12 O3 Si)x
CI PMS, COM
PCT Polyether, Polyether only
```

And an SRU for the ladder type if a RSiO1.5 unit is given

E.g.: RN 153315-80-1



Summary – polysiloxanes in REGISTRY

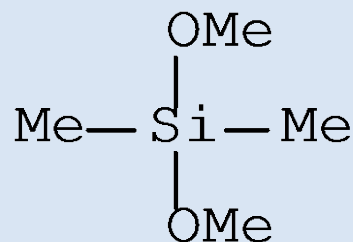
- Since 6/94, **hydrolytically prepared polysiloxanes** are treated as any other polymer being indexed as monomer-based entries or SRUs where appropriate.
- Prior to 6/94, **hydrolytically prepared polysiloxanes** were indexed at the controlled term “Siloxane and Silicones” with **NO CAS RN for the polymer**. The monomers were indexed with RNs with “D” appended and the type of polysiloxane in the textual information.
- The Registry entry for the product of **hydrolytic polymerization of halosilanes** includes **water as one component**.
- The Registry entry for the product of **hydrolytic polymerization of alkoxysilanes** does **NOT** include **water as one component**.

Polysiloxane search example

Search Question:

Find references to polydimethoxydimethylsilane

Dimethoxydimethylsilane:



Search for the RN of the monomer

=> E DIMETHOXYDIMETHYLSILANE/CN

E1 1 DIMETHOXYDIMETHYLOLTRIAZONE/CN
E2 1 DIMETHOXYDIMETHYLPHOSPHONIUM/CN
E3 1 --> DIMETHOXYDIMETHYLSILANE/CN

. . . .

=> S E3

L1 1 DIMETHOXYDIMETHYLSILANE/CN

=> D IDE

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2013 ACS on STN

RN 1112-39-6 REGISTRY

ED Entered STN: 16 Nov 1984

CN **Silane, dimethoxydimethyl-** (CA INDEX NAME)

OTHER NAMES:

CN AY 43-004

CN D 1052

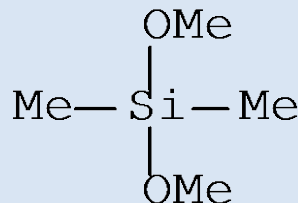
CN **Dimethoxydimethylsilane**

CN Dimethyldimethoxysilane

. . . .

MF C4 H12 O2 si

CI COM



Search for the homopolymer

```
=> S 1112-39-6/CRN AND 1/NC
L2          1 1112-39-6/CRN AND 1/NC
```

```
=> D IDE
```

```
L2  ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2013 ACS on STN
RN  25498-04-8  REGISTRY
ED  Entered STN:  16 Nov 1984
CN  Silane, dimethoxydimethyl-, homopolymer (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN  Silane, dimethoxydimethyl-, polymers (8CI)
OTHER NAMES:
CN  Dimethoxydimethylsilane homopolymer
CN  Dimethyldimethoxysilane homopolymer
CN  Dimethyldimethoxysilane polymer
CN  Dimethyldimethoxysilane-hexamethyldisiloxane copolymer
CN  Poly(dimethoxydimethylsilane)
DR  273209-60-2
MF  (C4 H12 O2 Si)x
CI  PMS
PCT Polyother, Polyother only
SR  CA
. . . .
```

A simple way to find the homopolymer is to search the monomer RN as a component registry number (/CRN).

Use POLYLINK to find related polymers

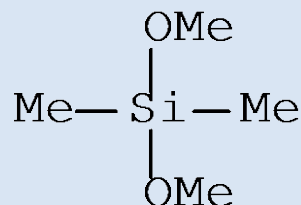
. . . .

****RELATED POLYMERS AVAILABLE WITH POLYLINK****

CM 1

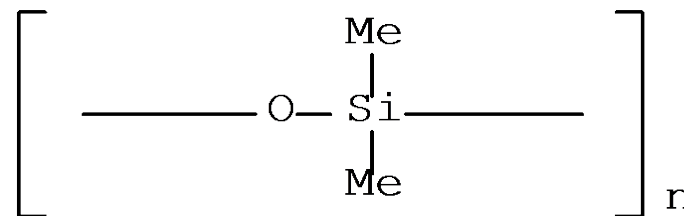
CRN 1112-39-6

CMF C4 H12 O2 si



Condensation polymerization of different monomers can lead to the same polymer. Monomer-based entries receive different RNs.

SRU based polymer RNs also exist for the polymer (different monomers can form the same SRU).



Use POLYLINK to find related polymers

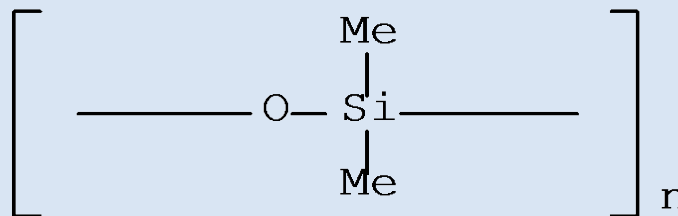
```
=> POLYLINK 25498-04-8  
L3          39 POLYLINK 25498-04-8
```

```
=> D IDE 1-39
```

```
. . . .
```

POLYLINK can find related SRU-based records, e.g.:

```
L3  ANSWER ... OF 39  REGISTRY  COPYRIGHT 2013 ACS on STN  
RN  9016-00-6  REGISTRY  
ED  Entered STN:  16 Nov 1984  
CN  Poly[oxy(dimethylsilylene)]  (CA INDEX NAME)  
. . . .  
MF  (C2 H6 O Si)n  
CI  PMS, COM  
PCT  Polyether, Polyether only  
. . . .
```



Use POLYLINK to find related polymers

And the same homopolymer made from other monomers, e.g.:

```
L3 ANSWER ... OF 39 REGISTRY COPYRIGHT 2013 ACS on STN
RN 1385013-20-6 REGISTRY
ED Entered STN: 01 Aug 2012
CN Silane, dimethyldipropoxy-, homopolymer (CA INDEX NAME)
. . .
```

```
L3 ANSWER ... OF 39 REGISTRY COPYRIGHT 2013 ACS on STN
RN 158158-00-0 REGISTRY
ED Entered STN: 07 Oct 1994
CN Silane, dichlorodimethyl-, homopolymer, hydrolytic (CA INDEX NAME)
. . .
```

```
L3 ANSWER ... OF 39 REGISTRY COPYRIGHT 2013 ACS on STN
RN 31900-57-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Silanediol, 1,1-dimethyl-, homopolymer (CA INDEX NAME)
. . .
```

```
L3 ANSWER ... OF 39 REGISTRY COPYRIGHT 2013 ACS on STN
RN 25037-57-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cyclotetrasiloxane, 2,2,4,4,6,6,8,8-octamethyl-, homopolymer
. . .
```

Retrieve references in CAplus

=> FILE HCAPLUS

=> S L2 AND P/DT

L4 76 L2 AND P/DT

=> D HITIND

L4 ANSWER ... OF 76 HCAPLUS COPYRIGHT 2013 ACS on STN

IPCI C08G0077-06 [I]; C08G0077-16 [I]

IPCR C08G0077-06 [I]; C08G0077-16 [I]

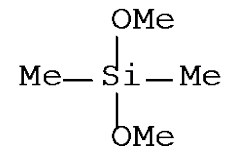
CC 35-5 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 37, 38

IT **25498-04-8P**, Dimethyldimethoxysilane homopolymer

RL: IMF (Industrial manufacture); PRP (Properties); PREP (Preparation)
(hydroxy-terminated; production of linear hydroxy-terminated
polydimethylsiloxanes via polycondensation of
dimethyldialkoxysilanes in active medium)

Patent references (L4) indexed with
dimethyldimethoxysilane homopolymer
(RN 25498-04-8) (L2).



Retrieve references in CPlus (cont.)

=> S L3 AND P/DT

L5 23527 L3 AND P/DT

Patent references (L5) indexed with any of the POLYLINK polydimethylsiloxane SRU or monomer-based RNs (L3).

=> D HITIND

L5 ANSWER ... OF 23527 HCAPLUS COPYRIGHT 2013 ACS on STN

IPCI D06M0013-328 [I]; D06M0013-463 [I]; D06M0013-144 [I]; D06M0013-12 [I];
D06M0015-643 [I]; D06M0015-647 [I]

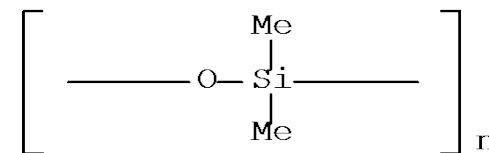
CC 46-5 (Surface Active Agents and Detergents)

Section cross-reference(s): 40, 23

IT **31900-57-9**, Polydimethylsiloxane

RL: MOA (Modifier or additive use); USES (Uses)

(emulsion containing, assumed monomers; softening agent emulsion-filled bags)



DWPI Polymer Indexing (1993-)

- In-depth indexing covering important polymer related information from DWPI basic patents
 - Both generic and specific concepts are indexed
- The codes provide additional information not present in the DWPI abstract
 - Generates unique hits compared to text searching, IPCs, etc.
- Searchable by subscribers*
 - Using the /PLE field, in either WPIDS or WPIX

(* An appropriate level of Thomson Reuters subscription is required.)

Example: DWPI polymer indexing

```
L1 ANSWER 1 OF 1 WPIX COPYRIGHT 2013 THOMSON REUTERS on STN
AN 1996-094459 [199610] WPIX
TI IR rays emitting material of good emission - covered with film
containing particles of oxide of one of iron, manganese and cobalt in
siloxane polymer
DC A26; A82; G02; P28; P42; X25
IN KATAYAMA S; KUBO Y; SAWADA I; YOSHINAGA I
PA (YAWA-C) NIPPON STEEL CORP
CYC 1
PIA JP 08003517 A 19960109 (199610)
ADT JP 08003517 A JP 1994-140549 19940622
PRAI JP 1994-140549 19940622
PLE UPA 20050511
[1.1] 018 D11 D10; O- 6A Ti 4B Tr Zr Ta 5B Nb Y- 3B Co 8B Gm;
H0260; P1445-R F81 Si 4A; M9999 M2108 M2095; L9999 L2391;
L9999 L2108 L2095; P1854;
[1.2] 018 D11 D10; P1912 D01 Al 3A O- 6A; H0260; P1445-R F81 Si
4A; M9999 M2108 M2095; L9999 L2391; L9999 L2108 L2095;
[1.3] 018 G2277-R G2266 D01 Si 4A D11 D10 D84 D85 D86 D87 D88 D89
D90 D91 D92 D93 F86 F87 G2288 G2277; G2277 G2266 D01 D11 D10
D50 D84 F86 F87 DCN: R23114 DCR: 1983; P1445-R F81 Si 4A;
P1456 P1445 F81 F86 D01 D11 D50 D82 Si 4A; H0000; H0022
H0011; L9999 L2573 L2506; L9999 L2528 L2506; L9999 L2664
L2506; M9999 M2108 M2095; L9999 L2391; L9999 L2108 L2095;
L9999 L2313; L9999 L2777;
[1.4] 018 ND01; K9836 K9790; Q9999 Q7669; Q9999 Q7705 Q7681; B9999
B5561 B5505; B9999 B5301 B5298 B5276; B9999 B3601 B3554;
Q9999 Q7114-R; K9610 K9483; K9712 K9676; N9999 N7147 . . .
```

DWPI polymer indexing is searched
and displayed using the **PLE** field.

Precision with three levels of linking

- **Level 3: Widest level – a “Linking group”**
 - Links related substances together
 - e.g. polymer with additive(s) or catalyst(s)
 - Links the polymer with properties and applications
- **Level 2: Middle level – indexing for each substance**
 - Links monomer and related terms within a polymer
 - Links a polymer to modified polymer terms
 - Links a compound with its function, shape or form
- **Level 1: Tightest level – Chemical Aspect (fragment) codes**
 - Links structural fragments together within a substance

Three linking operators on STN

Linking level

- (3) (widest)
- (2) (middle)
- (1) (tightest)

Proximity operator

- (L) Linking Group
- (P) Paragraph
- (S) Sentence

For example:

```
PLE  UPA  20050511
(L)  [1.1]  (P)  018 D11 D10; O- 6A Ti 4B Tr Zr Ta 5B Nb Y- 3B Co 8B Gm;
      [1.2]  018 D11 D10; P1445-R F81 Si 4A; M9999 M2108 M2095; L9999 L2391;
      [1.4]  018 ND01; K9836 K9790; Q9999 Q7669; Q9999 Q7705 Q7681; B9999
      B5561 B5505; B9999 B5301 B5298 B5276; B9999 B3601 B3554;
      Q9999 Q7114-R; K9610 K9483; K9712 K9676; N9999 N7147 . . .
```

DWPI polymer type codes (/PLE)

- P1445 Polysiloxane
 - P1456 NT Polydimethylsiloxane
 - P8184 NT Polymethylvinylsiloxane (2004-)
 - P8195 NT Polymethylphenylsiloxane (2004-)
 - P8208 NT Polyhydrogenmethylsiloxane (2004-)
 - P8219 NT Polysilsesquioxanes (2004-)

Hint: Searching [P1445/PLE](#) retrieves all narrower terms (NT).

- Also available:
 - P1423 Polysilane; P1434 Polysilazane.

Relevant monomer codes (/PLE)

- G2277 NT Si compounds containing 1 Si
 - R16680 NT Dimethylchlorosilane
 - R00383 NT Dimethyldichlorosilane
 - R24030 NT Methylchlorosilane
 - R00382 NT Trimethylchlorosilane
 - R24031 NT Methylmethoxysilane
 - R23114 NT Dimethyldimethoxysilane
 - R08655 NT Methyltrimethoxysilane
 - R09202 NT Methyltriethoxysilane (1996-)
 - R22582 NT Butyl methyl dimethoxysilane, t-
 - R08200 NT Diphenyldimethoxysilane
 - R00384 NT Methyltrichlorosilane
 - G2288 NT Si compounds containing 1 Si, other

Hint: Searching [G2277/PLE](#) retrieves all narrower terms (NT).

Relevant monomer codes* (/PLE) (cont.)

- G2299 NT Si compounds containing 2 Si or more
 - R04617 NT Hexamethyldisilazane
 - R07702 NT Octamethylcyclotetrasiloxane
 - G2302 NT Si compounds containing 2 Si or more, other

Hint: Searching [G2299/PLE](#) retrieves all narrower terms (NT).

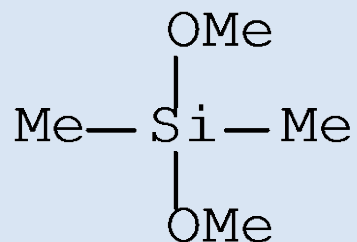
* Pages 23-24 of the DWPI Polymer Indexing Hierarchy:
http://www.stn-international.com/polymer_indexing_user_guides.html

Polysiloxane search example

Recall the Search Question:

Find references to polydimethoxydimethylsilane

Dimethoxydimethylsilane:



Search for the homopolymer

=> FILE WPIX*

=> S (R23114 (P) H0000)/PLE

L1 56 (R23114 (P) H0000)/PLE

=> D AN TI HITPLE

L1 ANSWER ... OF 56 WPIX COPYRIGHT 2013 THOMSON REUTERS on STN
AN 2007-254649 [200725] WPIX
TI Manufacture of alkyl siloxane aerogel useful as heat-insulating material, involves drying gel at temperature and pressure lower than critical point of solvent used for drying of gel
PLE UPA 20070417
[1.2] 2004 G2277 G2266 D01 D11 D10 D50 D84 F86 F87 DCN: R23114
DCR: 1983; P1456 P1445 F81 F86 D01 D10 D11 D50 D82 Si 4A;
H0000; L9999 L2573 L2506; S9999 S1365; S9999 S1309-R; L9999
L2313;

R23114 = dimethoxydimethylsilane
H0000 = homopolymer
(P) = link monomers and related terms within a polymer.

P1456 Polydimethylsiloxane.

(* An appropriate level of Thomson Reuters subscription is required.)

Search for the polymer type

=> FILE WPIX

=> S P1456/PLE

L1 23777 P1456/PLE

P1456 = polydimethylsiloxane.

=> D AN TI HITPLE

L1 ANSWER ... OF 23777 WPIX COPYRIGHT 2013

THOMSON REUTERS on STN

AN 2013-L62977 [201346] WPIX

TI Liquid composition, used as lipgloss for making up and/or caring of lips, comprises e.g. water, alkylcellulose, first non-volatile hydrocarbon oil including e.g. monomer and second non-volatile hydrocarbon oil including e.g. fluoro oil

PLE UPA 20130724

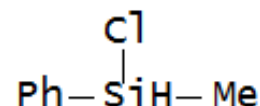
[1.1] 2004 P1456 P1445 F81 F86 D01 D10 D11 D50 D82 Si 4A; M9999 M2391;

Note: there are no “assumed monomers” in DWPI polysiloxane indexing.

An example using (L), (P) and (S)

Example:

Find references to methylphenylchlorosilane polysiloxanes used in coatings:



L1: (G2288 (S) F85 (S) F86 (S) D11 (S) D19 (S) D31 (S) D50 (S) D87 (S) Cl) /PLE

L2: L1 (P) P1445 /PLE

L3: L2 (L) Q7114 /PLE

G2288 = Si compounds containing 1 Si, other

F85 = Si-Halogen bond

F86 = Si-C bond

D11 = Aliphatic saturated chain

D19 = Benzene ring

D31 = 1 ring

D50 = No unsaturation

D87 = Carbon count 7 C

Cl = Chlorine

P1445 = Polysiloxane

Q7114 = Coatings

Note: as there is no specific code for methylphenylchlorosilane, a string of chemical aspect (fragment) codes are used to search for the substance.

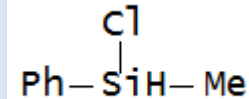
An example using (L), (P) and (S) (cont.)

=> S (G2288(S)F85(S)F86(S)D11(S)D19(S)D31(S)D50(S)D87(S)CL)/PLE
 L1 86 (G2288(S)F85(S)F86(S)D11(S)D19(S)D31(S)D50(S)D87(S)CL)/PLE

=> S L1 (P) P1445/PLE
 L2 38 L1 (P) P1445/PLE

=> S L2 (L) Q7114/PLE
 L3 11 L2 (L) Q7114/PLE

P1445 = Polysiloxane.
 Q7114 = Coatings.



=> D AN TI HITPLE

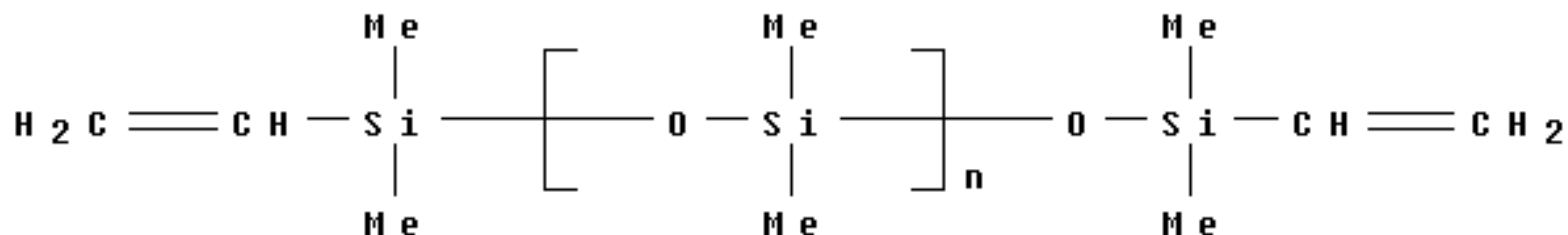
L3 ANSWER ... OF 11 WPIX COPYRIGHT 2013 THOMSON REUTERS on STN
 AN 2008-M13098 [200872] WPIX
 TI Metal anticorrosion treatment involves hydrolyzing silane coupling reagent with three alkyls in acid or alkaline environment to prepare silanol monomer and then polymerizing to obtain polymer (S)
 PLE UPA 20081110

(L) { [1.4] (P) { 2004 G2288 G2277 G2266 D01 Si 4A D11 D10 D19 D18 D31 D76 D50 D87 F85 F86 Cl 7A; H0000; P1445-R F81 Si 4A; L9999 L2313;
 [1.11] 2004 ND01; N9999 N7067 N7034 N7023; N9999 N7147 N7034 N7023; B9999 B5447 B5414 B5403 B5276; K9552 K9483; Q9999 Q7136 Q7114; ND07; ND03; N9999 N7045 N7034 N7023; B9999 B4591 B4568; B9999 B4488 B4466; B9999 B4477 B4466; K9905;

Single-unit polysiloxane SRUs with end groups

Recall the example:

A polysiloxane with an author representation:



Indexed with the given SRU:

Either (P1456 (P) H0395)/PLE, and/or (P1456 (P) M2813 (P) M2153)/PLE

P1456 = Polydimethylsiloxane

H0395 = Unsaturation end functional polymer

M2813 = Unsaturation incorporated polymer

M2153 = End group modified polymer

No assumed monomer indexing!

Multi-unit polysiloxane SRUs

Recall the example:

A polysiloxane represented by the author as $(-\text{OSiMe}_2)_x(-\text{OSiPh}_2)_y$ with no preparative information given.

Indexed with the given SRU:

For example: (P1445 (P) D92 (P) D19 (P) D32 (P) D50 (P) D82 (P) D11) /PLE

P1445 = Polysiloxane

D92 = Carbon count 12 C

D19 = Benzene ring

D32 = 2 rings

F86 = Si-C bond

D50 = No unsaturation

D82 = Carbon count 2 C

D11 = Aliphatic saturated chain

$(-\text{OSiPh}_2)_y$

$(-\text{OSiMe}_2)_x$

No assumed monomer indexing!

A note on DWPI Plasdoc Coding (1966-1994)

- Key Serial (/KS)
 - 1306: Polysiloxane (silicone) (1978-1994)
- Section A multi-punch (AM) code (/FG)
 - 38-: Polysiloxane (silicone) (1966-1994)

```
=> S 1306/KS OR 38-/FG
1306 Siloxanes
L1      71446 1306/KS OR 38-/FG
```

Use "Plasdoc Coding" to search for polysiloxanes prior to 1995.

```
=> D AN TI HIT
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L1      ANSWER ... OF 71446  WPIX COPYRIGHT 2013          THOMSON REUTERS on STN
AN      1994-366280 [199445]  WPIX
TI      Target for white balancing endoscopic camera - is silicone-titanium
        di:oxide body providing uniform diffused light to probe tip
PLC     UPA      20050701
        KS: 0009 0072 0075 0078 0147 0149 0150 0152 0153 0155 0165 0168 0205
           0218 0231 1303 1306 2014 2016 2020 2021 2208 2211 2220 2299 2321
           2706 2768 2851 3258
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. . . .
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A note on DWPI Manual Codes (/MC)

- A06-A SILICON POLYMERS

including silicones, polysiloxanes, polysilazanes

- A06-A00A . Production
- A06-A00B . Compositions
- A06-A00C . Fabrication
- A06-A00D . Treatment
- A06-A00E . Uses
 - A06-A00E1 .. Adhesives and binders; coatings, textile treatment (1970-)
 - A06-A00E2 .. Chemical, electrical and mechanical engineering (1970-)
 - A06-A00E3 .. Medical, dental, cosmetic and veterinary (1986-)
 - A06-A00E4 .. (Electro)photographic; printing; optical (1986-)

A note on DWPI Manual Codes (/MC) (cont.)

- B04-C03F – Silicones (pharmaceutical.) (2005-)
- C04-C03F – Silicones (agrochem./vet.) (2005-)

=> FILE WPIX

=> S (A06-A00E3 OR B04-C03F OR C04-C03F)/MC

L1 15993 (A06-A00E3 OR B04-C03F OR C04-C03F)/MC

=> D TI MC 1-20

L1 ANSWER ... OF 15993 WPIX COPYRIGHT 2013 THOMSON REUTERS on STN
TI Non-aqueous oral care composition for whitening a tooth, comprises a peroxide component, and an adhesion system comprising a hydrophobic component comprising a silicone adhesive, and a dental surface adhesion enhancing agent

MC CPI: A06-A00E3; A12-V04B; D08-B08

L1 ANSWER ... OF 15993 WPIX COPYRIGHT 2013 THOMSON REUTERS on STN
TI Oral syrup composition based on simeticone, sorbitol, potassium citrate, vitamin B1 and B6 used for the adjuvant treatment of functional dyspeptic symptomatology

MC CPI: B04-C03F; B10-A07B; B10-C02; B12-M07; B12-M12N; B14-E01; B15-B01; B15-B06

DWPI Chemistry Resource (DCR)

- DCR is a database of specific substances indexed in Derwent World Patents Index (DWPI)
- While DCR is not used to routinely index patents classified in Section A (Polymers), there are some polymer substance records available to pharmaceutical and chemical (BCE) indexers
- Polysiloxane and oligosiloxane substances (of chemical/pharmaceutical interest) are assigned the DCR substance descriptor “silicones”, i.e.

=> **S SILICONES/CC**

Polysiloxanes in DCR

=> FILE WPINDEX

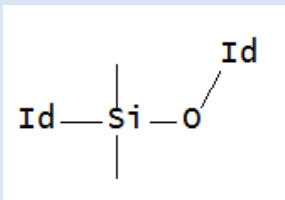
=> S SILICONES/CC

L1 114 SILICONES/CC

Retrieve DCR substance records (L1).

=> D ALL

L1 ANSWER ... OF 114 WPINDEX COPYRIGHT 2013 THOMSON REUTERS on STN
AN.S DCR-114171
DCSE 114171-0-0-0
CN.P DIMETICONE
SY DIMETHICONE; DIMETHYLPOLYSILOXANE; DIMETHYLSILICONE;



CMT A polymer containing dimethylsiloxane, $\text{OSi}(\text{CH}_3)_2$ Standard polymer
MF Polymer
SDCN R08017; RA09KM
CC POLYMERS; SILICONES

=> S L1/DCR

L2 12470 L1/DCR

Retrieve DWPI patent records (L2).

Summary

- Types of silicon polymers
- Polysiloxanes in CAplus/REGISTRY
 - Alkoxysilane-based polysiloxanes
 - Halosilane-based polysiloxanes
 - Polysiloxanes prepared by ring-opening polymerization
 - Single-unit polysiloxane SRUs
 - Multi-unit polysiloxane SRUs
 - Silsesquioxanes
- Polysiloxanes in DWPI Polymer Indexing
- Polysiloxanes in DWPI Chemistry Resource (DCR)

Acknowledgement

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