

Searching for Polymer Information on STN[®]

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Overview of the Guide

Introduction

This guide is intended to facilitate the retrieval of polymer information in STN databases (or “files”). It is assumed that you are experienced in STN search and retrieval techniques.

For additional information about searching STN, refer to STN Support & Training pages at www.cas.org.

Structure of this guide

The Guide is structured as follows:

- **Chapter 1** provides an overview of polymer information available on STN and defines polymer terminology.
 - **Chapter 2** describes registration, assignment of CAS Registry Numbers[®], and content of polymer records in the CAS REGISTRYSM database.
 - **Chapter 3** describes search strategies for finding CAS Registry Numbers for polymers in REGISTRY.
 - **Chapter 4** describes polymer subject indexing terms in the CASM/CAplusSM database.
 - **Chapter 5** provides an overview of polymer searching in non-CAS databases on STN.
-

Chapter 1

Overview of Polymer Information on STN

Introduction

Polymer information is found throughout STN in virtually every database. From the perspective of the polymer scientist, some databases will be of far greater interest than others, but relevant information on polymers and applications may be found almost anywhere in STN. This guide is aimed at assisting the polymer searcher in retrieving polymer information of interest from the most likely source databases.

Polymer information

Most papers dealing specifically with polymers are concerned about:

- Starting monomers
 - Final polymer structure
 - Post-treatment
 - Polymer chemistry and properties
 - Processing of polymers
 - Polymer applications
 - Polymer compositions and formulations
 - Plastics manufacture and processing
-

Polymers in REGISTRY and CAplus

REGISTRY is the world's largest and most current source of CAS Registry Numbers (CAS RNs) for polymers that can be used in other databases to locate literature references for specific polymers. In databases that do not contain CAS RNs, REGISTRY provides polymer names for use in your searches.

REGISTRY has:

- More than 1 million polymeric substance records
- Daily updating with new polymer entries
- A unique CAS RN for each polymer record

Most of these polymer records are linked to references in CAplus.

Polymer cluster The polymer database cluster in STN consists of the databases with significant amounts of polymer information.

=> **D CLU POLYMERS**

CLUSTER NAME	CLUSTER DEFINITION
POLYMERS	APOLLIT BABS CAPLUS CBNB CIN COMPENDEX DISSABS EMA IFIPAT NTIS PASCAL PROMT RAPRA SCISEARCH TEXTILETECH USPATFULL USPATOLD USPAT2 WPIDS WPIFV WPINDEX WSCA WTEXTILES Polymer Science Cluster

The STN Database Summary Sheets for these databases may be viewed at www.cas.org.

Polymer definition and terminology

A polymer is a naturally occurring or synthetic macromolecule formed by linking together smaller molecules (monomers). REGISTRY also identifies smaller “mers”, e.g., dimmers, trimers, tetramers. By definition, polymers contain 10 or more monomer units. The polymer terms and their definitions are shown in this table.

Term	Definition	Example
Homopolymer	Polymer formed from a single monomer	Polytetrafluoroethylene MF = (C ₂ F ₄) _x
Copolymer	Polymer formed from two or more monomers	Styrene, polymer with ethene MF = (C ₈ H ₈ .C ₂ H ₄) _x
Addition (Vinyl) Polymer	Polymer formed through chain reaction in which one monomer is added to another	Styrene, polymer with ethene MF = (C ₈ H ₈ .C ₂ H ₄) _x
Condensation Polymer	Polymer formed by loss of a simple molecule such as water	1,4-butanediol-phthalic acid copolymer MF = (C ₈ H ₆ O ₄ .C ₄ H ₁₀ O ₂) _x
Structural Repeating Unit (SRU)	Smallest structural unit that can repeat in the polymer backbone	Poly(butylene phthalate) MF = (C ₁₂ H ₁₂ O ₄) _n
Post-Treated Polymer	Polymer that is modified either partially or completely, after the basic polymer backbone has formed	Sulfonated polystyrene
Tacticity	The stereoregularity of the polymer	
Block Polymer	Polymers where the monomers are arranged in blocks	-AAAA-BBBB- (A and B are monomers)
Alternating Polymer	Polymers where the monomers alternate regularly	-A-B-A-B-A-B-A-B-
Graft Polymers	Polymers where the main backbone has attached to it macromolecular side chains of a different set of monomers	<p style="text-align: center;">B-B-B-B-</p> <p style="text-align: center;"> </p> <p>-A-A-A-A-A-A-A-A-</p>
Polymer Blend	Homogeneous or heterogeneous physical mixture of two or more polymers	
Composite	Systems including a polymer matrix and a dispersed phase	Glass-fiber reinforced polyester
Cross-linking Agents	Multifunctional materials providing cross-linking bridges in a polymer network	

Chapter 2

Polymers in REGISTRY

Overview

Introduction This chapter provides information on polymer registration, assignment of CAS RNs, and content of records in REGISTRY.

Contents This chapter contains the following sections:

- Overview of polymer registration by CAS
- Monomer-based registration
- Supplementary registration using structural repeating units
- Exceptions to monomer-based registration
- Polymers with specific tacticity
- Block, graft, and alternating copolymers
- Incompletely identified polymers

Polymer Registration by CAS

Polymer Class Identifiers

Substances that are registered as polymers have the entry POLYMER and PMS in the Class Identifier (CI) field. These are:

- Polymeric substances with 11 or more repeating units
- Oligomers with an unknown or fractional number of monomer units or with 10 or less monomer units, if the exact structure is unknown (e.g., 1-Hexene, trimer CAS RN 72607-62-6)

```
CN 1-Hexene, trimer (CA INDEX NAME)
MF (C6 H12)3
CI PMS
```

CAS RN assignment

Each record is identified by a unique CAS Registry Number based on the monomer(s) actually used to form the polymer. Additional CAS RNs may be assigned to structural repeating units (SRUs).

Separate CAS RNs are not assigned for:

- Head-to-tail or head-to-head polymers
- Linear or branched polymers
- Polymer blends
- Most post-treated polymers

The above information may often be found in the CPlus index entry with the polymer CAS RN.

Post-treated polymers that do get their own CAS RN are:

- Salts of polymers such as metal salts, amine salts, or hydrochlorides

```
RN 1092479-21-4 REGISTRY
CN 2-Propenoic acid, 2-methyl-, 2-(dimethylamino)ethyl
ester, polymer with 2-methyloxirane, triblock,
hydrochloride (CA INDEX NAME)
```

- Polymer esters and polymer ethers

```
CN 1,4-Dioxane-2,5-dione, 3,6-dimethyl-, (3S,6S)-,
polymer with oxirane, ester with 2,2-
bis(hydroxymethyl)-1,3-propanediol (4:1), tetramethyl
ether, diblock (CA INDEX NAME)
```

- Addition compounds, e.g. quaternized polymers

```
CN 2,5-Furandione, polymer with ethenylbenzene,
2-[(2-hydroxyethyl)amino]ethyl ester, alternating,
ammonium salt, compd. with 2,2'-iminobis[ethanol]
(CA INDEX NAME)
```

**Information
excluded from
REGISTRY
records**

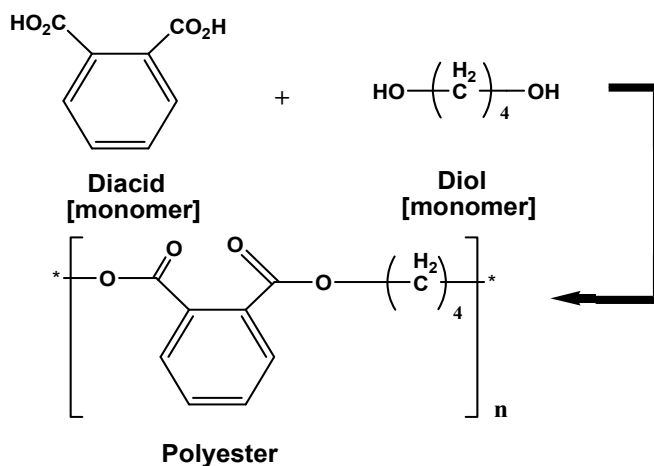
REGISTRY records for polymers do not include:

- Other substances that participate in the polymerization process, e.g., chain initiators and polymerization catalysts
 - Ratios between the monomers
 - Number of repeating units in the polymer backbone
 - Molecular weight of the polymer
 - Presence or absence of end groups for monomer-based polymer records
-

Monomer-Based Registration

Monomer definition

The *primary* way a polymer is structured and registered in REGISTRY is based on the *monomers making up the polymer*. A monomer is any multifunctional substance that is incorporated into the polymer through polymerization or cross-linking.



Definition of fields in the example record

The principal parts of the monomer-based record are:

- 1 CAS RN for the polymer
 - 2 Systematic CA Index name [(9CI) refers to the version of CA Index nomenclature used for the name (1972 rules).]
 - 3 Molecular Formula: two component formulas separated by a period and enclosed in parentheses with an "x" subscript to indicate the polymer
 - 4 Polymer Class Terms (PCTs)
 - 5 Locator (LC) field: listing other STN databases where this polymer is indexed by its CAS RN
 - 6 POLYLINK command: enabling the linking of related polymers
 - 7 Each component (CM) monomer: displayed with its CAS RN, molecular formula, and structure
 - 8 References in CA and CPlus
-

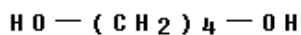
Example of a monomer-based polymer record

The CAS Registry Number is the database key for the REGISTRY record. CAS RNs are assigned to the polymer and to the monomers.

RN 26352-63-6 REGISTRY ①
ED Entered STN: 16 Nov 1984
CN 1,2-Benzenedicarboxylic acid, polymer with 1,4-butanediol
(CA INDEX NAME) ②
OTHER CA INDEX NAMES:
CN 1,4-Butanediol, polyester with phthalic acid (8CI)
CN 1,4-Butanediol, polymer with 1,2-benzenedicarboxylic acid
(9CI)
CN Phthalic acid, polyester with 1,4-butanediol (8CI)
OTHER NAMES:
CN 1,4-Butanediol-phthalic acid copolymer
CN Poly(butylene phthalate)
MF (C8 H6 O4 . C4 H10 O2)x ③
CI PMS
PCT Polyester, Polyester formed ④
LC STN Files: CA, CAPLUS, CHEMLIST, IFICDB, IFIPAT,
IFIUDB, TOXCENTER, USPAT2, USPATFULL USPATOLD ⑤
RELATED POLYMERS AVAILABLE WITH POLYLINK ⑥

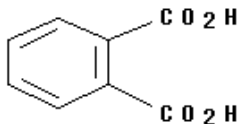
CM 1

CRN 110-63-4 ⑦
CMF C4 H10 O2



CM 2

CRN 88-99-3
CMF C8 H6 O4



57 REFERENCES IN FILE CA (1907 TO DATE) ⑧
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
57 REFERENCES IN FILE CAPLUS (1907 TO DATE)

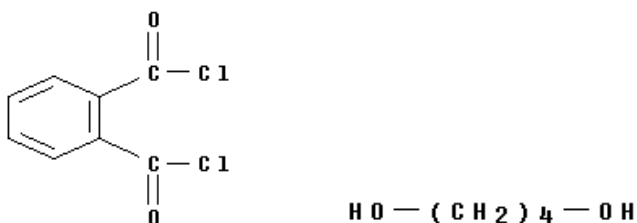
**Additional
monomer-
based records**

The polyester formed by the acid and alcohol monomers shown can also be prepared from other sets of monomers. Each of these different sets of monomers receives a different CAS RN even though they all result in the same final polymer. Two examples (partial records) are shown below for:

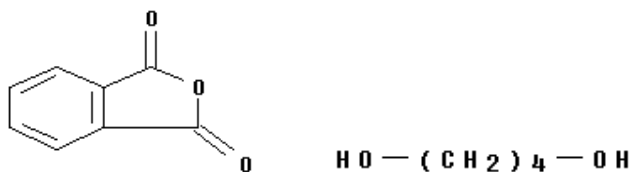
- Diacid halide and diol
- Acid anhydride and diol

Other sets of monomers could have been used to prepare this polyester. Using the POLYLINK command identifies all such polymers that have been entered into REGISTRY.

```
RN 86889-85-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,2-Benzenedicarbonyl dichloride, polymer with 1,4-
   butanediol (9CI) (CA INDEX NAME)
MF (C8 H4 Cl2 O2 . C4 H10 O2)x
```



```
RN 32472-86-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1,3-Isobenzofurandione, polymer with 1,4-butanediol (9CI)
   (CA INDEX NAME)
MF (C8 H4 O3 . C4 H10 O2)x
```

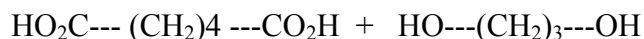


Supplementary Registration Using Structural Repeating Units

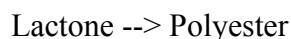
Rules

In addition to the monomer-based representations, an additional record with its own CAS RN is created in REGISTRY for the *structural repeating unit* (SRU) of the polymer in the following cases:

- **Condensation** polymers from **2 symmetrical** monomers.



- Ring-opening polymerization if only one final structure is possible.



- The author stresses the SRU and provides supporting evidence for its structure.

SRU entries are rarely made for addition polymers.

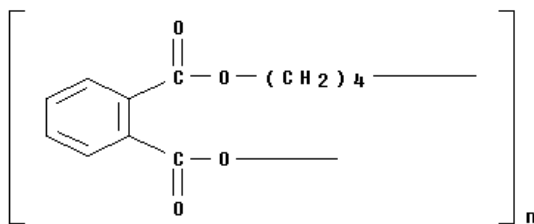
Assignment of CAS RNs

The SRU entry gets a different CAS RN than the monomer-based entries.

```
RN 26499-89-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Poly(oxycarbonyl-1,2-phenylenecarboxyloxy-1,4-butanediyl)
   (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Poly(oxyphthaloyloxytetramethylene) (8CI)
OTHER NAMES:
CN 1,4-Butanediol-phthalic acid copolymer, SRU
CN 1,4-Butanediol-phthalic anhydride copolymer, sru
CN 1,4-Butanediol-phthaloyl chloride copolymer, sru
CN Phthalic anhydride-THF copolymer, SRU
CN Poly(butylene phthalate), SRU
MF (C12 H12 O4)n
CI PMS
PCT Polyester
LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB,
   TOXCENTER, USPAT2, USPATFULL, USPATOLD
```

RELATED POLYMERS AVAILABLE WITH POLYLINK

(Continued on the next page)



53 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 53 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Appearance of SRU records

The SRU record has some differences from monomer-based records:

- Different CAS RN
- Repeating unit name
- Single component formula with “n” subscript instead of “x”
- Polymer backbone structure

End groups

Most SRUs do not have end groups specified as part of their structure. The remaining SRUs do have end groups. Separate CAS RNs are assigned for each case.

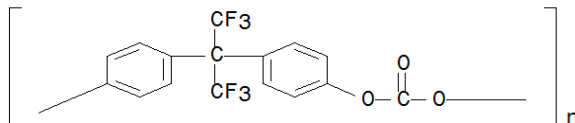
SRU without end groups

```
RN 32291-26-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN Poly[oxy-carbonyloxy-1,4-phenylene[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]-1,4-phenylene] (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Poly[oxy-carbonyloxy-p-phenylene[trifluoro-1-(trifluoromethyl)ethylidene]-p-phenylene] (8CI)
OTHER NAMES:
CN 1,1,1,3,3,3-Hexafluoro-2,2-bis(4-hydroxyphenyl)propane-phosgene copolymer,
sru
CN 2,2-Bis(4-hydroxyphenyl)-1,1,1,3,3,3-hexafluoropropane-phosgene copolymer,
SRU
CN 4,4'-(Hexafluoroisopropylidene)bisphenol bis(chloroformate) homopolymer,
sru
CN Bisphenol AF polycarbonate sru
CN Bisphenol AF-phosgene copolymer, SRU
CN Bisphenol AF-trichloromethyl chloroformate copolymer, sru
CN Carbonic acid-hexafluorobisphenol A copolymer, sru
DR 156147-43-2
MF (C16 H8 F6 O3)n
```

(Continued on the next page)

CI PMS
PCT Polycarbonate
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL

RELATED POLYMERS AVAILABLE WITH POLYLINK

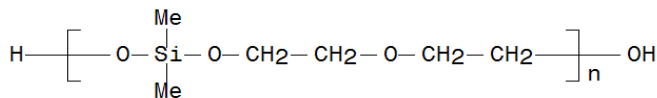


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

76 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
76 REFERENCES IN FILE CAPLUS (1907 TO DATE)

SRU with end groups

RN 31242-71-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Poly[oxy(dimethylsilylene)oxy-1,2-ethanediyl]oxy-1,2-ethanediyl, .alpha.-hydro-.omega.-hydroxy- (9CI)
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Poly[oxy(dimethylsilylene)oxyethyleneoxyethylene], .alpha.-hydro-.omega.-hydroxy- (8CI)
MF (C6 H14 O3 Si)n H2 O
CI PMS
PCT Polyether



Exceptions to Monomer-Based Registration

List of exceptions

There are four exceptions to the monomer-based rule for registration:

- Five common polymers normally indexed only at their SRU
 - Polymer structure too large¹ or unknown
 - Polymer identified only by a trade name
 - Polymer indexed only as a concept,² i.e., a controlled vocabulary index heading in the CA/CAPLUS database
-

Very common polymers

Certain very common polymers are indexed **only** at the SRU entry in CAPLUS unless they are prepared from non-standard monomers:

Nylon 6	RN 25038-54-4
Nylon 66	RN 32131-17-2
PEG (polyethylene glycol)	RN 25322-68-3
PPG (polypropylene glycol)	RN 25322-69-4
PET (poly(ethylene terephthalate))	RN 25038-59-9

Polymer too large or unknown

If the structure of the polymer is too large or is not known, no structure is available in the REGISTRY record. One example is a copolymer with very many different monomer components.

```
RN 153699-89-9 REGISTRY
ED Entered STN: 18 Mar 1994
CN 1,3-Benzenedicarboxylic acid, polymer with 1,4-
benzenedicarboxylic acid, Burnock D 750, 1,4-butanediol,
2-butyl-2-ethyl-1,3-propanediol, butyl 2-methyl-2-
propenoate, 1,4-dihydroxy-2-butanedisulfonic acid
monosodium salt, 1,6-diisocyanatohexane, 1,3-
diisocyanatomethylbenzene, 2-(dimethylamino)ethyl 2-
methyl-2-propenoate, 2,2-dimethyl-1,3-propanediol, 1,2-
ethanediol, ethenylbenzene, 2-ethylhexyl 2-methyl-2-
propenoate, hexanedioic acid, 2-hydroxyethyl 2-methyl-2-
propenoate, methyl 2-methyl-2-propenoate, 2-methyl-2-[(1-
oxo-2-propenyl)amino]-1-propanedisulfonic acid monosodium
salt and 2-methyl-2-propenoic acid (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Ethanediol, polymer contg. (9CI)
MF Unspecified
CI PMS, MAN
PCT Manual registration
SR CA
LC STN Files: CA, CAPLUS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)
```

¹ These may be indexed in terms of the monomers, but there is no monomer structure.

² Beginning in 1994, there are far fewer such cases.

**Identified only
by a trade
name**

If the polymer is only identified by a trade name with no known structure or a partially known structure, no monomer-based registration can be created. The polymer gets a “manual registration.” (Note the MF and PCT.)

```
RN 1048665-85-5  REGISTRY
ED Entered STN:  11 Sep 2008
CN Biocycle 2000-0  (CA INDEX NAME)
ENTE A hydroxybutyric acid polymer (PHB Industries)
MF Unspecified
CI PMS, MAN
PCT Manual registration
SR CA
LC STN Files:  CA, CAPLUS
```

```
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
      3 REFERENCES IN FILE CA (1907 TO DATE)
      3 REFERENCES IN FILE CAPLUS (1907 TO DATE)
```

The editing note (ENTE) indicates all CAS knows about Biocycle 2000-0.

**Indexed as a
concept**

In some cases, the polymer may be indexed in CA/CAPLUS only as a subject indexing term and not as a substance with a CAS RN.

For example, certain rubbers (prior to 1987) and fibers (prior to 1992) were indexed **only** at a subject heading in CAPLUS. No CAS RNs were used. Since that time, CAS RNs for many, but not all, of the rubber and fiber index entries back to 1967 have been added.

A comprehensive search strategy may not be easily devised by the novice polymer searcher, so consulting an experienced polymer searcher is advisable.

The CA Lexicon in CAPLUS alerts searchers to existing and previous indexing policies.

```
=> E POLYESTER FIBERS+HNTE,NOTE/CT
E1 75982 --> Polyester fibers/CT
           HNTE Valid heading during volume 76 (1972)
           to present.
           NOTE Fibers from all polyesters and
           polythioesters are indexed here.
***** END *****
```

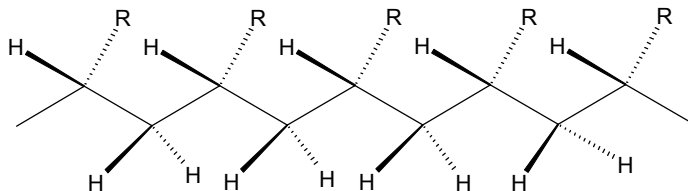
Polymers with Specific Tacticity

Tacticity definitions

Tacticity is the stereoregularity of the substituent groups on the polymer backbone. Each form gets a separate CAS RN.

Isotactic example

Isotactic (all substituents on same side of backbone):



RN 55929-71-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Hexene, polymer with 1-propene, isotactic (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Propene, polymer with 1-hexene, isotactic (9CI)
OTHER NAMES:
CN 1-Hexene-propylene isotactic copolymer
CN Isotactic 1-hexene-propene copolymer
CN Isotactic 1-hexene-propylene copolymer
CN Isotactic propylene-1-hexene polymer
CN Propylene-1-hexene isotactic copolymer
MF (C6 H12 . C3 H6)x
CI PMS
PCT Polyolefin
LC STN Files: CA, CAPLUS, CHEMLIST, IFICDB, IFIPAT, IFIUDB, USPATFULL

CM 1

CRN 592-41-6

CMF C6 H12

H₂C=CH-Bu-n

CM 2

CRN 115-07-1

CMF C3 H6

H₃C-CH=CH₂

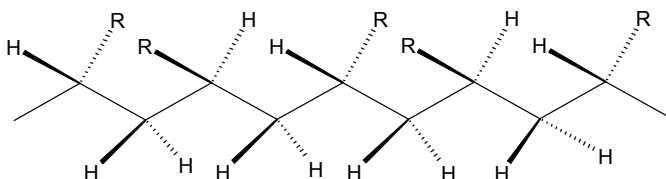
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

26 REFERENCES IN FILE CA (1907 TO DATE)

26 REFERENCES IN FILE CAPLUS (1907 TO DATE)

**Syndiotactic
example**

Syndiotactic (alternating arrangement of substituents):



RN 133006-21-0 REGISTRY
ED Entered STN: 05 Apr 1991
CN 1-Hexene, polymer with 1-propene, syndiotactic (CA INDEX
NAME)
OTHER CA INDEX NAMES:
CN 1-Propene, polymer with 1-hexene, syndiotactic (9CI)
OTHER NAMES:
CN 1-Hexene-propylene copolymer, syndiotactic
CN 1-Hexene-propylene syndiotactic copolymer
CN Syndiotactic 1-hexene-propylene copolymer
MF (C6 H12 . C3 H6)x
CI PMS
PCT Polyolefin
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 592-41-6
CMF C6 H12

H₂C=CH-Bu-n

CM 2

CRN 115-07-1
CMF C3 H6

H₃C-CH=CH₂

10 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Atatic example Atactic (irregular or unknown arrangement of substituents; if no tacticity is specified, atactic is assumed):

RN 25895-44-7 REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Hexene, polymer with 1-propene (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Hexene, polymer with propene (8CI)
CN 1-Propene, polymer with 1-hexene (9CI)
CN Propene, polymer with 1-hexene (8CI)
OTHER NAMES:
CN 1-Hexene-propene copolymer
CN 1-Hexene-propene polymer
CN 1-Hexene-propylene copolymer
CN 1-Hexene-propylene polymer
CN Eastoflex D 127
CN Propene-1-hexene copolymer
CN Propylene-1-hexene copolymer
CN TX 1771-131
MF (C6 H12 . C3 H6)x
CI PMS, COM
PCT Polyolefin
LC STN Files: CA, CAPLUS, CASREACT, CHEMLIST, IFICDB,
IFIPAT, IFIUDB,
TOXCENTER, USPAT2, USPATFULL, USPATOLD

CM 1

CRN 592-41-6

CMF C6 H12

$\text{H}_2\text{C}=\text{CH}-\text{Bu}-\text{n}$

CM 2

CRN 115-07-1

CMF C3 H6

$\text{H}_3\text{C}-\text{CH}=\text{CH}_2$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

294 REFERENCES IN FILE CA (1907 TO DATE)
18 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
294 REFERENCES IN FILE CAPLUS (1907 TO DATE)

**Other
stereoregular
terms**

There are other stereoregular terms associated with polymers, e.g., threo-diisotactic, meso-diisotactic, erythro-diisotactic, racemo-diisotactic, threo-disyndiotactic, meso-disyndiotactic, erythro-disyndiotactic, and racemo-disyndiotactic. Polymers with these tacticities also receive separate CAS RNs.

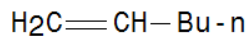
Block, Graft, and Alternating Copolymers

Assignment of CAS RNs Block polymers in records from 1982 to the present receive their own CAS RNs and are identified with a more precise, searchable chemical name segment: diblock, triblock, tetrablock, or pentablock.

RN 850562-36-6 REGISTRY
ED Entered STN: 17 May 2005
CN 1-Hexene, polymer with 1-propene, triblock (CA INDEX
NAME)
OTHER NAMES:
CN 1-Hexene-propylene triblock copolymer
MF (C6 H12 . C3 H6)x
CI PMS
PCT Polyolefin
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

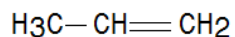
CM 1

CRN 592-41-6
CMF C6 H12



CM 2

CRN 115-07-1
CMF C3 H6



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

**Indexing at
plain polymer**

Prior to 1987, block, graft, and alternating copolymers were indexed at the CAS RN for the “plain” polymer with terms such as “block” or “graft” in the modifying phrase following the CAS RN in CPlus. Records from 1967 to 1986 are being enhanced with the addition of block CAS RNs.

**Block polymer
search strategy**

A search of the three block polymer CAS RNs in CPlus for the 1-hexene 1-propene copolymer yields 12 retrievals.

```
=> S (181961-64-8 OR 755025-68-4 OR 850562-36-6)
L4          12 S(181961-64-8 OR 755025-68-4 OR 850562-36-6)
```

Coincidentally, a search of the “plain” copolymer CAS RN with the block terms also retrieves 12 hits.

```
L8          12 S 25895-44-7 (L) (BLOCK OR DIBLOCK OR TRIBLOCK)
```

The two searches combined gives 21 hits.

```
=> S 14 or 18
L9          21 L4 OR L8
```

Incompletely Identified Polymers

Polymers with incomplete information

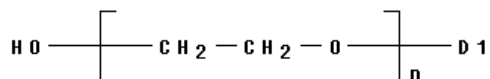
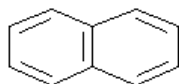
For some polymers, some of the monomers are specific structures while others may be incomplete or have unknown structures. Two types of cases are illustrated:

- Incompletely described substances
 - EPDM (ethylene-propylene-diene monomer) polymers
-

IDS polymers

There are many incompletely described substances (IDS) in REGISTRY. Some are also polymers.

RN 69778-08-1 REGISTRY
ED Entered STN: 16 Nov 1984
CN Poly(oxy-1,2-ethanediyl), α -naphthalenyl- ω -hydroxy- (CA INDEX NAME)
OTHER NAMES:
CN Newcol B 13
CN Newcol NN 15
CN Newcol NS 20
CN Polyethylene glycol mononaphthyl ether
CN Polyethylene oxide mononaphthyl ether
DR 83856-15-9
MF (C2 H4 O)_n C10 H8 O
CI IDS, PMS, COM
PCT Polyether
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



114 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
115 REFERENCES IN FILE CAPLUS (1907 TO DATE)

In this polymer, the location of the naphthalenyl attachment is unknown.

**EPDM
polymers that
are rubbers**

EDPM rubber is an index heading in CAplus.

IT EPDM rubber
RL: POF (Polymer in formulation); TEM (Technical or
engineered material use); USES (Uses)
(fire-, heat-, and voltage-resistant halogen-free
polyolefin compns. for elec. wire jackets)

The Lexicon entry shows the current policy:

E8 9212 --> EPDM rubber/CT
HNTE Valid heading during volume 126 (1997) to
present.
NOTE Ethylene-propylene-nonconjugated diene
copolymer.
E9 OLD Rubber, synthetic (L) EPDM/CT

**Diene monomer
known**

When the diene monomer is specified, an entry is made both at the copolymer
RN and the index heading.

IT **25034-77-9**, Ethylene-methylenenorbornene-propene
copolymer
RL: PEP (Physical, engineering or chemical process); PYP
(Physical process); PROC (Process)
(rubber; producing bales of EPDM rubbers with low
levels of dusting agent from pellets)
IT EPDM rubber
RL: PEP (Physical, engineering or chemical process); PYP
(Physical process); PROC (Process)
(ethylene-methylenenorbornene-propene, Vistalon 5600,
Vistalon 7000; producing bales of EPDM rubbers with
low levels of dusting agent from pellets)

**EPDM with no
CAS RN**

EPDM (pre-1997) is indexed with no CAS RN when the diene was unknown.

IT Synthetic rubber, uses
RL: MOA (Modifier or additive use); USES (Uses)
(EPDM, fracture and morphol. of polypropylene/EPDM
blends)

**EPDM indexing
1977-present**

Since 1997, EPDM rubber with the diene unknown is indexed in CAplus at the CAS RNs for the known monomers with "D" and/or "DP" appended to the CAS RN to indicate derivatives. (Non-specific derivatives do not get a separate CAS RN in REGISTRY.)

IT **74-85-1D**, Ethylene, polymers with propylene and dienes
115-07-1D,
Propylene, polymers with ethylene and dienes
RL: POF (Polymer in formulation); TEM (Technical or
engineered material use); USES (Uses)
(rubber; fire-, heat-, and voltage-resistant halogen-
free polyolefin compns. for elec. wire jackets)

IT EPDM rubber
Polyolefins
RL: POF (Polymer in formulation); TEM (Technical or
engineered material use); USES (Uses)
(fire-, heat-, and voltage-resistant halogen-free
polyolefin compns. for elec. wire jackets)

Chapter 3

Search Strategies in REGISTRY

Overview

Introduction

Begin your polymer search in REGISTRY. Once the polymers of interest have been found, the L-number(s) may then be crossed into CAplus to retrieve the relevant references. Append the L-number by /D to search for non-specific derivatives.

Types of searches

REGISTRY offers a number of alternatives for polymer searching. The following are discussed in this chapter:

- Name searching
 - Component CAS RN searching
 - POLYLINK to find all related condensation polymers
 - Polymer Class Term searching
 - Structure searching
-

Name Searching

Overview of name searching

Search in the Basic Index, Chemical Name (/CN), or the Chemical Name Segment (/CNS) fields. Search for:

- Monomer names
 - Polymer names
 - Trade names
-

Monomer name search

This approach is useful when you know the monomer name(s). Use EXPAND to verify search terms prior to searching. Use (L) proximity to link the monomer names. Use both ?POLY?/CNS and PMS/CI to limit the search to polymers.

```
=> S STYRENE (L) ACRYLIC ACID AND (?POLY?/CNS OR PMS/CI)
L5      8997 STYRENE (L) ACRYLIC ACID AND (?POLY?/CNS OR PMS/CI)
```

Polymer name search

Use hyphens to separate the monomer names (preferably in alphabetic order) in the polymer and EXPAND in the /CN field, and then search E3 if it is present.

```
=> E ACRYLIC ACID-METHYL METHACRYLATE-STYRENE COPOLYMER/CN 5
E1      1      ACRYLIC ACID-METHYL METHACRYLATE-STYRENE BLOCK
          COPOLYMER/CN
E2      1      ACRYLIC ACID-METHYL METHACRYLATE-STYRENE BLOCK
          GRAFT COPOLYMER/CN
E3      1 --> ACRYLIC ACID-METHYL METHACRYLATE-STYRENE
          COPOLYMER/CN
E4      1      ACRYLIC ACID-METHYL METHACRYLATE-STYRENE
          COPOLYMER
          2-(DIMETHYLAMINO)ETHANOL SALT/CN
E5      1      ACRYLIC ACID-METHYL METHACRYLATE-STYRENE
          COPOLYMER CALCIUM AND SODIUM SALT/CN
```

```
=> S E3
```

Polymer names may also begin with "Poly". Again, verify name with EXPAND in the /CN field.

```
=> S POLYETHYLENE/CN
L1      1 POLYETHYLENE/CN
```

```
=> S "POLY (HEXAFLUORO-1,3-BUTADIENE) "/CN
L3      1 "POLY (HEXAFLUORO-1,3-BUTADIENE) "/CN
```

Trade name search

When searching a trade name, be sure to look for variations in spelling and punctuation.

```
=> S SARAN SL 159/CN
L3          1 SARAN SL 159/CN
```

Be alert to ambiguous trade names or acronyms, e.g., PET.

Component CAS Registry Number Searching

Component CAS RN search

Search the CAS RN for each monomer in the Component Registry Number (CRN) field. Link multiple CAS RNs using AND operators. Specify the number of components in the /NC numeric field.

```
=> S 95-13-6/CRN AND 80-62-6/CRN AND NC>2
L1          15 95-13-6/CRN AND 80-62-6/CRN AND NC>2
```

POLYLINK Command

POLYLINK

The same polymer may be created from several different sets of monomers. In a monomer-based registration, each set of monomers will have a separate CAS RN. In addition, condensation polymers, e.g., polyamides, polycarbonates, may be registered and indexed on the basis of their SRUs. Comprehensive searching requires finding all such registrations.

With the POLYLINK command, you can retrieve the CAS RNs for the monomer-based and structural repeating unit representations for a given condensation polymer or a set of polymers.

POLYLINK may be used on:

- An individual CAS Registry Number
 - Any REGISTRY answer set, an E-number list, or an ANALYZE list of CAS Registry Numbers
-

**POLYLINK
example**

For example, the polymer formed between 1,4-butanediol and terephthalic acid may also be formed in various ways. If you know the CAS RN for one of the records (26062-94-2 in this example), you can easily find all related CAS RNs.

=> **POLYLINK 26062-94-2**

L2 17 POLYLINK 26062-94-2

There are 16 different monomer-based registrations and one SRU registration covering this polymer.

=> **D SCAN CN**

L2 17 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,4-Benzenedicarboxylic acid, bis(4-hydroxybutyl) ester,
 polymer with 1,4-benzenedicarbonyl dichloride (9CI)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1) :**16**

L5 17 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,4-Benzenedicarboxylic acid, bis(4-hydroxybutyl) ester,
 homopolymer (9CI)

• • •

L5 17 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,4-Benzenedicarboxylic acid, dicesium salt, polymer with
 1,4-dibromobutane (9CI)

L5 17 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,4-Benzenedicarboxylic acid, bis(2-hydroxyethyl) ester,
 polymer with 1,4-butanediol (9CI)

L5 17 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,4-Benzenedicarboxylic acid, polymer with 1,4-butanediol
 and 1,4-dimethyl 1,4-benzenedicarboxylate

L5 17 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN 1,4-Benzenedicarboxylic acid, 1,4-dimethyl ester, polymer
 with 1,4-butanediol

L5 17 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Poly(oxy-1,4-butanediylloxycarbonyl-1,4-phenylenecarbonyl)
 ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT

ALL ANSWERS HAVE BEEN SCANNED

Polymer Class Terms

Assignment of Polymer Class Terms

Polymer Class Terms (PCTs) categorize the various polymers in REGISTRY into 42 classes. For many categories, there is also a FORMED subcategory where the linkage is formed as part of the polymerization. PCTs are assigned to all polymers except oligomers (dimers, trimers, tetramers, etc.) and coordination compound polymers that would only receive the class POLYOTHER or one of the MANUAL class terms. If the classification for a polymer is uncertain, it receives the class POLYOTHER.

Polymer class terms are assigned algorithmically. Each term represents the structural characteristics of the polymer backbone and reflects:

- The types of linkages formed in the polymerization process
 - Linkages already present within the monomer backbone
 - Linkages present in structural repeating unit (SRU) backbones
-

FORMED

If, when assigning the polymer class terms, the system identifies that a linkage for a certain class was formed during the polymerization process, a second polymer class term with the word FORMED added is indexed. When you search a class term without the word FORMED, you also retrieve the FORMED polymers. FORMED terms are present for all classes except resins, addition polymers, double stranded polymers, and polynucleotides.

PCT list

AMINO RESIN	POLYCARBODIIMIDE	POLYPHENYL
CHLOROPOLYMER	POLYCARBODIIMIDE FORMED	POLYPHENYL FORMED
DOUBLE STRAND	POLYCARBONATE	POLYPHOSPHAZENE
EPOXY RESIN	POLYCARBONATE FORMED	POLYPHOSPHAZENE FORMED
FLUOROPOLYMER	POLYCYANURATE	POLYQUINOXALINE
MANUAL COMPONENT	POLYCYANURATE FORMED	POLYQUINOXALINE FORMED
MANUAL REGISTRATION	POLYESTER	POLYSTYRENE
PHENOLIC RESIN	POLYESTER FORMED	POLYSULFIDE
POLYACETYLENE	POLYETHER	POLYSULFIDE FORMED
POLYACRYLIC	POLYETHER FORMED	POLYSULFONAMIDE
POLYAMIC ACID	POLYHYDRAZIDE	POLYSULFONAMIDE FORMED
POLYAMIC ACID FORMED	POLYHYDRAZIDE FORMED	POLYSULFONE
POLYAMIDE	POLYIMIDE	POLYSULFONE FORMED
POLYAMIDE FORMED	POLYIMIDE FORMED	POLYTHIOESTER
POLYAMINE	POLYIONENE	POLYTHIOESTER FORMED
POLYAMINE FORMED	POLYIONENE FORMED	POLYTHIOETHER
POLYANHYDRIDE	POLYISOCYANURATE	POLYTHIOETHER FORMED
POLYANHYDRIDE FORMED	POLYISOCYANURATE FORMED	POLYUREA
POLYAZOMETHINE	POLYKETONE	POLYUREA FORMED
POLYAZOMETHINE FORMED	POLYKETONE FORMED	POLYURETHANE
POLYBENZIMIDAZOLE	POLYNUCLEOTIDE	POLYURETHANE FORMED
POLYBENZIMIDAZOLE FORMED	POLYOLEFIN	POLYVINYL
POLYBENZOXAZOLE	POLYOTHER	
POLYBENZOXAZOLE FORMED	POLYOTHER ONLY	

PCT search examples

Combine the PCT term(s) with other search terms using AND/NOT operators.

PCT and name term:

```
=> S ?POLYPROPYLENE?/CNS AND POLYETHER/PCT AND POLYSULFONE/PCT
      4213 ?POLYPROPYLENE?/CNS
      317652 POLYETHER/PCT
      19006 POLYSULFONE/PCT
L4      11 ?POLYPROPYLENE?/CNS AND POLYETHER/PCT AND
      POLYSULFONE/PCT
```

=> D 6

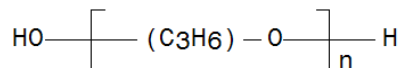
```
L4 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2009 ACS on STN
RN 865188-03-0 REGISTRY
ED Entered STN: 13 Oct 2005
CN 1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-, polymer with
.alpha.-hydro-.omega.-hydroxypoly[oxy(methyl-1,2-
ethanediyl)], 5-isocyanato-1-(isocyanatomethyl)-1,3,3-
trimethylcyclohexane and 4,4'-sulfonylbis[benzenamine]
(9CI) (CA INDEX NAME)
```

OTHER NAMES:

```
CN 4,4'-Diaminodiphenyl sulfone-isophorone diisocyanate-
polypropylene glycol-trimethylolpropane copolymer
MF (C12 H18 N2 O2 . C12 H12 N2 O2 S . C6 H14 O3 .
(C3 H6 O)n H2 O)x
CI PMS
PCT Polyether, Polysulfone, Polyurea, Polyurea formed,
Polyurethane, Polyurethane formed
SR CA
LC STN Files: CA, CAPLUS
```

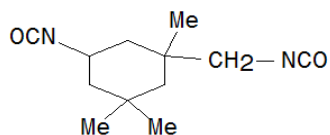
CM 1

```
CRN 25322-69-4
CMF (C3 H6 O)n H2 O
CCI IDS, PMS
```



CM 2

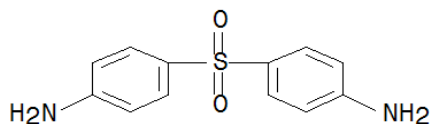
```
CRN 4098-71-9
CMF C12 H18 N2 O2
```



(Continued on next page)

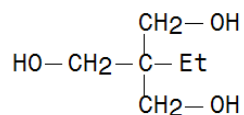
CM 3

CRN 80-08-0
CMF C12 H12 N2 O2 S



CM 4

CRN 77-99-6
CMF C6 H14 O3



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

PCT and CAS RN:

=> S 80-05-7/CRN AND POLYETHER FORMED/PCT AND POLYURETHANE/PCT

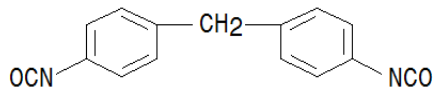
30727 80-05-7/CRN
87468 POLYETHER FORMED/PCT
83716 POLYURETHANE/PCT

L1 299 80-05-7/CRN AND POLYETHER FORMED/PCT AND
POLYURETHANE/PCT

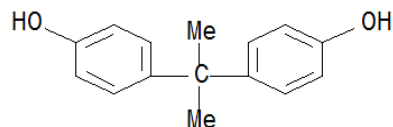
=> D SCAN

L1 299 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
IN Phenol, 4,4'-(1-methylethylidene)bis-, polymer with
1,1'-methylenebis[4-isocyanatobenzene], methyloxirane and
oxirane, block (9CI)
MF (C15 H16 O2 . C15 H10 N2 O2 . C3 H6 O . C2 H4 O)x
CI PMS

CM 1

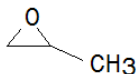


CM 2



(Continued on next page)

CM 3



CM 4



**PCT as a subset
for structure
searching**

PCT searches provide excellent answer sets for use in subset structure searches. For example, find polyureas containing fluorine where the polyurea is formed during the polymerization.

=> **S POLYUREA FORMED/PCT**

L1 20503 POLYUREA FORMED/PCT

L2 STRUCTURE UPLOADED

=> **S L2 SUB=L1 FUL**

FULL SUBSET SEARCH INITIATED 08:09:38

FULL SUBSET SCREEN SEARCH COMPLETED - 664 TO ITERATE

100.0% PROCESSED 664 ITERATIONS

68 ANSWERS

SEARCH TIME: 00.00.01

L3 68 SEA SUB=L1 SSS FUL L2

=> **D**

L3 ANSWER 1 OF 68 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1133960-69-6 REGISTRY

ED Entered STN: 13 Apr 2009

CN Urea, N,N''-9H-fluorene-2,7-diylbis[N'-(3-aminopropyl)-,
polymer with N,N'-bis(5-isocyanato-3-pyridinyl)urea (CA
INDEX NAME)

MF (C21 H28 N6 O2 . C13 H8 N6 O3)x

CI PMS

PCT Polyurea, Polyurea formed

SR CA

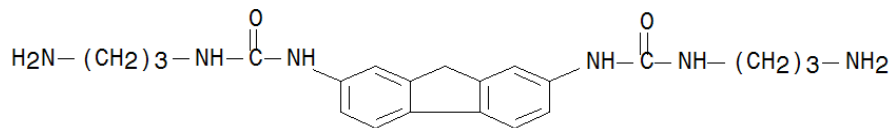
LC STN Files: CA, CAPLUS

RELATED POLYMERS AVAILABLE WITH POLYLINK

CM 1

CRN 1133960-68-5

CMF C21 H28 N6 O2

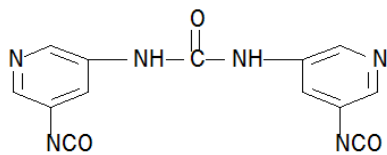


(Continued on next page)

CM 2

CRN 1133960-65-2

CMF C13 H8 N6 O3



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Structure Searching

Structure searching

Structure searching for monomers in polymers is no different than other structure searching. To limit the search to polymers only, polymer screens (filters) may be added. This may be done with the SCREEN command online or using the structure drawing tools in STN Express[®] or STN[®] on the WebSM.

Polymer screens

The polymer screens are:

- 2043 Any polymer with a structure or a manual CAS RN
 - 2067 Homopolymer or copolymer (non-SRU)
 - 2068 Any SRU
 - 2069 SRU with end groups
 - 2070 SRU without end groups
-

Copolymer search strategy

The search strategy for structure searching for a copolymer is:

Step	Action
1	Draw a separate fragment for each monomer (probably not more than four).
2	Use the SCREEN command for the polymer screen (non-SRU). => SCR 2067 L1
3	Upload each fragment into a REGISTRY session. => Uploading ... L2 STRUCTURE UPLOADED => Uploading ... L3 STRUCTURE UPLOADED ...
4	Run a SAMPLE SEARCH. => S (L2 AND L3) AND L1
5	Review answers.
6	Run FULL search. => S L4 FUL FULL SEARCH INITIATED 13:02:46 FULL SCREEN SEARCH COMPLETED - 144 TO ITERATE 100.0% PROCESSED 144 ITERATIONS 34 ANSWERS SEARCH TIME: 00.00.01 L5 34 SEA SSS FUL (L1 AND L2) AND L3

7

Display answers.

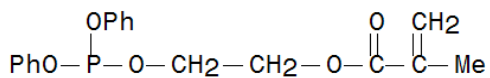
=> D

L5 ANSWER 1 OF 34 REGISTRY COPYRIGHT 2009 ACS on
STN
RN 1146851-81-1 REGISTRY
ED Entered STN: 14 May 2009
CN INDEX NAME NOT YET ASSIGNED
MF (C18 H19 O5 P . C5 H8 O2 . C4 H6 O2 . (C3 H6 O)n
C18 H26 O2)x
CI PMS
PCT Polyacrylic, Polyether
SR CA
LC STN Files: CA, CAPLUS

•••

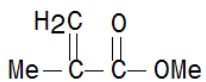
CM 2

CRN 24619-51-0
CMF C18 H19 O5 P



CM 3

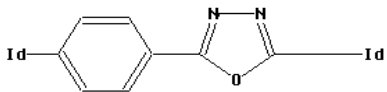
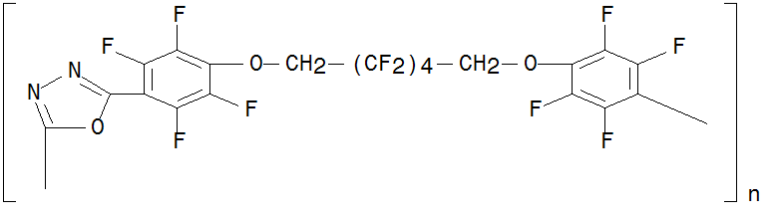
CRN 80-62-6
CMF C5 H8 O2



•••

**SRU without end groups:
search strategy**

The search strategy for structure searching for a SRU without end groups is (SAMPLE search omitted):

Step	Action
1	<p>Draw the SRU.</p>  <p>The "Id" dummy nodes are necessary to show the SRU end points. This example is for an SRU without end groups.</p>
2	<p>Retrieve structure matches for the SRU without end groups (screen 2070).</p> <pre> => SCR 2070 L1 SCREEN CREATED L2 STRUCTURE UPLOADED => S L2 AND L1 FUL FULL SEARCH INITIATED 12:35:18 FULL SCREEN SEARCH COMPLETED - 908 TO ITERATE 100.0% PROCESSED 908 ITERATIONS 276 ANSWERS SEARCH TIME: 00.00.01 L3 276 SEA SSS FUL L5 AND L1 => D L3 29 L7 ANSWER 29 OF 276 REGISTRY COPYRIGHT 2009 ACS on STN RN 1007089-63-5 REGISTRY ED Entered STN: 07 Mar 2008 CN Poly[1,3,4-oxadiazole-2,5-diyl(2,3,5,6- tetrafluoro-1,4-phenylene)oxy(2,2,3,3,4,4,5,5- octadecafluoro-1,6-hexanediyl)oxy(2,3,5,6- tetrafluoro-1,4-phenylene)] (CA INDEX NAME) MF (C20 H4 F16 N2 O3)n CI PMS PCT Polyether SR CA LC STN Files: CA, CAPLUS **RELATED POLYMERS AVAILABLE WITH POLYLINK** </pre>  <pre> 1 REFERENCES IN FILE CA (1907 TO DATE) 1 REFERENCES IN FILE CAPLUS (1907 TO DATE) </pre>

3

Use POLYLINK to retrieve related monomer-based polymer registrations.

=> **POLYLINK 1007089-63-5**

L8 2 POLYLINK 1007089-63-5

=> **D 2**

L8 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2009 ACS on STN

RN 1007089-62-4 REGISTRY

ED Entered STN: 07 Mar 2008

CN 1,6-Hexanediol, 2,2,3,3,4,4,5,5-octafluoro-, polymer with 2,5-bis(2,3,4,5,6-pentafluorophenyl)-1,3,4-oxadiazole (CA INDEX NAME)

MF (C14 F10 N2 O . C6 H6 F8 O2)x

CI PMS

PCT Polyether, Polyether formed

SR CA

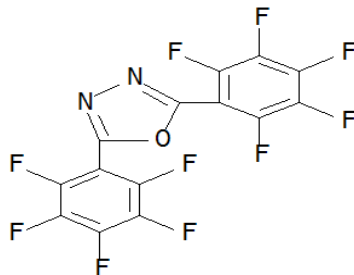
LC STN Files: CA, CAPLUS

RELATED POLYMERS AVAILABLE WITH POLYLINK

CM 1

CRN 16184-59-1

CMF C14 F10 N2 O



CM 2

CRN 355-74-8

CMF C6 H6 F8 O2

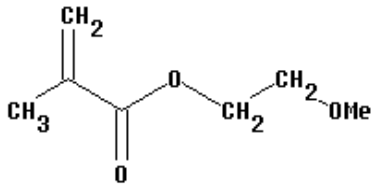
HO-CH₂-(CF₂)₄-CH₂-OH

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

SRU with end groups: search strategy

The search strategy for structure searching for a SRU with end groups is (SAMPLE search omitted):

Step	Action
1	<p>Draw the SRU with the end groups attached.</p>  <p>STN will identify the "O-CH2-CH2" repeating group.</p>
2	<p>Retrieve the matches for the SRU with the specified end groups using the query and screen 2069.</p> <pre> => SCR 2069 L1 SCREEN CREATED L2 STRUCTURE UPLOADED => S L2 AND L1 FULL FULL SEARCH INITIATED 08:23:57 FULL SCREEN SEARCH COMPLETED - 23371 TO ITERATE 100.0% PROCESSED 23371 ITERATIONS 4777 ANSWERS SEARCH TIME: 00.00.01 L3 4777 SEA SSS FUL L2 AND L1 </pre>
3	<p>Display answers.</p> <pre> RN 26915-72-0 REGISTRY ED Entered STN: 16 Nov 1984 CN Poly(oxy-1,2-ethanediyl), .alpha.-(2-methyl-1-oxo-2-propen-1-yl)-.omega.-methoxy- (CA INDEX NAME) OTHER CA INDEX NAMES: CN Glycols, polyethylene, monomethacrylate, methyl ether (8CI) CN Methacrylic acid, ester with polyethylene glycol methyl ether (8CI) OTHER NAMES: CN Bisomer 350 CN Bisomer MPEG 1000MA CN Bisomer MPEG 350MA CN Bisomer MPEG 550MA CN Bisomer S 10W CN Bisomer S 20W CN Bisomer S 7W CN Blemmer PME 1000 CN Blemmer PME 150 CN Blemmer PME 200 </pre> <p style="text-align: right;"><i>(Continued on next page)</i></p>

CN Blemmer PME 400
CN Blemmer PME 4000
CN Blemmer PME 450
CN Blemmer PME 550

•••

CN NK Ester M 230G

ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT - Use
FCN, FIDE, or ALL for DISPLAY

DR 862118-84-1, 876930-62-0, 1007311-66-1, 161161-
97-3, 122093-20-3, 133184-10-8, 96256-82-5,
104491-18-1, 106340-32-3, 115402-22-7,
136036-18-5, 112352-67-7, 138981-97-2, 139091-
15-9, 142233-43-0, 78623-21-9, 152730-80-8,
110540-42-6, 156932-34-2, 161126-65-4,
180028-35-7, 189638-26-4, 191940-85-9, 218956-
80-0, 220654-94-4, 256488-92-3, 292149-01-0

MF (C2 H4 O)n C5 H8 O2

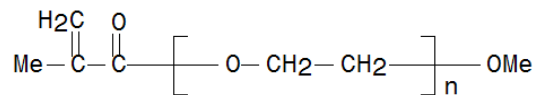
CI PMS, COM

PCT Polyether

LC STN Files: AGRICOLA, BIOSIS, CA, CAPLUS,
CASREACT, CHEMCATS, CHEMLIST, CSCHEM, IFICDB,
IFIPAT, IFIUDB, TOXCENTER, USPAT2, USPATFULL,
USPATOLD

Other Sources: NDSL**, TSCA**

(**Enter CHEMLIST File for up-to-date
regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

823 REFERENCES IN FILE CA (1907 TO DATE)

275 REFERENCES TO NON-SPECIFIC DERIVATIVES IN
FILE CA

826 REFERENCES IN FILE CAPLUS (1907 TO DATE)

Chapter 4

Using Polymer Subject Indexing Terms

Introduction Polymers are indexed in CAplus³ as CAS Registry Numbers and by using Controlled vocabulary (/CT) index entries for specific polymers or for polymer classes.

Chapter 3 discussed search strategies for finding CAS RNs in REGISTRY that you can then crossover as an L-number to CAplus.

This chapter focuses on using polymer subject indexing terms in CAplus.

Finding Controlled Terms (CTs) Policies for the assignment of Controlled Vocabulary (CT) indexing terms can change over time. The CA Lexicon in the /CT field of CA/CAplus can alert you to present and past indexing policies.

Use the EXPAND command in the usual way as well as with the CA Lexicon thesaurus in the /CT field. Enter HELP LEXICON in at an arrow prompt (=>) in CAplus for further details.

```
=> E RUBBER, BUTADIENE-STYRENE/CT
E#   FREQUENCY   AT   TERM
--   -
...
E3           107    2 --> RUBBER, BUTADIENE-STYRENE/CT
E4              0    2   RUBBER, BUTADIENE-STYRENE (L)
              (ANILINOPHENYL)METHACRYL AMIDE- AND
              (PHENYLTHIOETHYL) VINYL BENZENE-
              GRAFTED/CT
E5              0    2   RUBBER, BUTADIENE-STYRENE (L)
              ACRYLIC-GRAFTED/CT
E6              0    2   RUBBER, BUTADIENE-STYRENE (L) AMINE-
              TERMINATED/CT
E7              0    2   RUBBER, BUTADIENE-STYRENE (L)
              BLOCK/CT
...

```

The presence of the “AT” column indicates that the terms are in the CA Lexicon. The number of terms connected with the (L) operator should prompt us to search the /CT using truncation.

(continued on next page)

³ When searching using the CA Lexicon, it is recommended that the searches be done in the HCAPLUS database, which does not use search term pricing. In CAplus OR ZCAplus, Lexicon searches may become quite costly.

```
=> S RUBBER, BUTADIENE-STYRENE?/CT
L2      24536 RUBBER, BUTADIENE-STYRENE?/CT
```

The CA Lexicon shows current and past indexing practice.

```
=> E RUBBER, BUTADIENE-STYRENE+PFT,OLD/CT
E1      107    --> Rubber, butadiene-styrene/CT
E2      25454   NEW Styrene-butadiene rubber/CT
***** END *****
```

We can search on the current term and use the thesaurus to bring in other related terms in the search as well.

```
=> S E2+OLD, PFT, NT
L3      28228 "STYRENE-BUTADIENE RUBBER"+OLD, PFT, NT/CT
          (1417 TERMS)
```

Combine the two searches for the total result.

```
=> S L2 OR L3
L4      52470 L2 OR L3
```

```
=> D HIT 1 23500 HIT
```

```
L4 ANSWER 1 OF 52470 CAPLUS COPYRIGHT 2009 ACS on STN
IT Styrene-butadiene rubber
   RL: PEP (Physical, engineering or chemical process); PROC
       (Process)
       (Cariflex 1502, soln. rubber and vulcanizate surface;
        lowering friction of surfaces of rubber materials by
        treating surfaces with rubber solns. or latexes
        contg. graphite or molybdenum disulfide)
```

```
L4 ANSWER 23500 OF 52470 CAPLUS COPYRIGHT 2009 ACS on STN
IT Rubber, butadiene-styrene, uses
   RL: USES (Uses)
       (EPDM rubber blends, automotive glass runs,
        polyurethane abrasion-resistant coatings for)
```

Additional answers

Additional answers may be found using the CAS RN for the known butadiene-styrene copolymer or its non-specific derivatives.

=> **S 9003-55-8 (L) RUBBER**

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L6 49911 L5

L7 37152 L6 (L) RUBBER

=> **S L7 NOT L4**

L8 574 L7 NOT L4

=> **D HIT**

L8 ANSWER 1 OF 574 CAPLUS COPYRIGHT 2009 ACS on STN
IT **9003-55-8D**, Butadiene-styrene copolymer, acrylic modified
RL: POF (Polymer in formulation); TEM (Technical or engineered material use); USES (Uses)
(**rubber**; bottles having coatings contg. Interference pigments with unique and high-quality appearance)

Further answers may be obtained by considering specific derivatives of the butadiene-styrene copolymer.

=> **FIL REG**

=> **S (BUTADIENE STYRENE COPOLYMER) AND 2/NC**

L9 31 (BUTADIENE STYRENE COPOLYMER) AND 2/NC

=> **FIL HCAPLUS**

=> **S L9 (L) RUBBER**

L10 47091 L8 (L) RUBBER

=> **S L10 NOT (L4 OR L7)**

L11 661 L10 NOT (L4 OR L7)

**Polymer class
index terms**

Many index terms for polymer classes may be used in the /CT field.

IT Polyureas
Polyurethanes
RL: IMF (Industrial manufacture); POF (Polymer in
formulation); PREP (Preparation); USES (Uses)
(manuf. of polyurea- or polyurethane-alumina
nanocomposites)

**Searching for
rubbers**

Elastomers or rubbers are characterized by their ability to stretch or contract rapidly. Elastomers are obtained from natural sources and by synthetic means. A Controlled Term entry is made for the rubber regardless whether a CAS RN is also used.

**Indexing for
rubbers**

Rubber indexing policy:

E6 188181 --> Rubber/CT
HNTE Valid heading during volume 1 (1907) to
present.
NOTE Studies on elastomers or rubber of
unknown origin are indexed here. Studies on
elastomers or rubber of natural origin are
indexed at **Natural rubber** or its narrower
terms. Studies on elastomers or rubber of
synthetic origin are indexed at **Synthetic
rubber** or its narrower terms.

E7 6 OLD Elastomers/CT

**Rubber in the
CA Lexicon**

A search of “rubber” using the CA Lexicon terms retrieves many hits in
CAplus.

=> **S RUBBER+NT/CT**

L1 282106 RUBBER+NT/CT (32 TERMS)

=> **D HIT 1000**

L1 ANSWER 1000 OF 282106 HCAPLUS COPYRIGHT 2006 ACS on STN

IT **Silicone rubber, uses**

RL: DEV (Device component use); USES (Uses)
(XE 15 751, elastic layer; heating device using
flexible film with elastic layer and releasing layer
for electrophotog. app.)

Searching RUBBER/CW yields additional rubber retrievals, but not
everything the CA Lexicon terms found.

=> **S RUBBER/CW**

L2 285279 RUBBER/CW

=> **S L2 NOT L1**

L3 8876 L2 NOT L1

=> **D HIT 2000**

L3 ANSWER 2000 OF 8876 HCAPLUS COPYRIGHT 2006 ACS on STN

IT **Rubber**, substitute and synthetic

(from cyclopentadiene, 2,5-dimethyl-1,5-hexadiene,
isoprene and 2-methyl-1-butene, O3-resistant rapid-
curing)

The term “rubbers” also appears in the controlled indexing.

=> **S RUBBERS/CW**

L4 87880 RUBBERS/CW

=> **D 3000 HIT**

L4 ANSWER 3000 OF 87880 HCAPLUS COPYRIGHT 2006 ACS on STN

IT Extrusion apparatus for plastics and **rubbers**

(sizing core; sizing cores blowing cooling air for
plastic pipe extrusion with smooth inner walls)

IT Extrusion of plastics and **rubbers**

Pipes and Tubes

(sizing cores blowing cooling air for plastic pipe
extrusion with smooth inner walls)

Generic rubber searches

Generic searches for rubbers may be approached in several ways as the following examples illustrate.

Search the Basic Index (with plurals set on):

```
=> S RUBBER
      350607 RUBBER
      145635 RUBBERS
L1    424822 RUBBER
      (RUBBER OR RUBBERS)
```

The Controlled Words or the Lexicon provide more controlled results (index heading words only):

```
=> S RUBBER?/CW
L2    361203 RUBBER/CW

=> S RUBBER+PFT,NT/CT
L3    278856 RUBBER+PFT,NT/CT (48 TERMS)
```

The Controlled Term index entry itself still provides a large number of answers ranging in time from 1907 to the present.

```
=> S RUBBER/CT
L4    187652 RUBBER/CT (1 TERM)
```

Rubber uses and applications

Many of the common uses and applications of rubbers are indexed at the use. Often a separate index entry is made for the rubber.

```
IT    Gloves
      (manufg. method for injection molded rubber gloves
       with low cost and improved phys. property)
IT    Natural rubber
      Synthetic rubber
      RL: PEP (Physical, engineering or chemical process); PYP
      (Physical process); TEM (Technical or engineered material
      use); PROC (Process); USES (Uses)
      (manufg. method for injection molded rubber gloves
       with low cost and improved phys. property)
```

In other cases, no rubber term is indexed.

```
IT    Tires
      (treads, isoprene rubber compns. for, for low heat
      buildup and roll resistance and high skid resistance)
```

Chapter 5

Polymer Searching in non-CAS Databases

Introduction

Almost every STN database includes some polymer information. More than 20 databases have over 100,000 hits on the term POLYMER? in the Basic Index. In addition to standard search techniques, STN provides some special features to facilitate polymer searching:

- POLYMERS database cluster
 - INDEX command
 - CAS RN crossover
 - SELECT NAME and ANALYZE NAME
-

POLYMERS database cluster

The polymer science database cluster consists of:

```
=> D CLU POLYMERS
CLUSTER NAME          CLUSTER DEFINITION
-----
POLYMERS              APOLLIT BABS CAPLUS CBNB CIN COMPENDEX
                     DISSABS EMA IFIPAT NTIS PASCAL PROMT
                     RAPRA SCISEARCH TEXTILETECH USPATFULL
                     USPATOLD USPAT2 WPIDS WPIFV WPINDEX WSCA
                     WTEXTILES
                     Polymer Science Cluster
```

You may use the cluster with the FILE command or with STNINDEX.

SET CLUSTER

Users may create customized polymer database clusters using the SET CLUSTER command. Enter SET CLUSTER at an arrow prompt (=>) followed by the name of the cluster you want to create. Cluster names must:

1. Begin with a period (.)
2. Have 2-16 characters
3. Contain only letters A-Z, numbers (0-9), and periods (.)

You will be prompted to define the cluster. Enter one or more valid database names, user-defined clusters, system-defined clusters, or combinations of these. Separate the names with a space or a comma. The defined cluster is then saved permanently on your login ID.

```
=> SET CLUSTER
ENTER CLUSTER NAME OR (?): .MYCLUSTER
ENTER LIST OF FILE NAMES OR (?): CAPLUS BIOSIS
MORE FILES, (NONE), OR ?:.
CLUSTER '.MYCLUSTER' DEFINED AS 'CAPLUS, BIOSIS'
SET COMMAND COMPLETED
```

INDEX

The INDEX command may be used with the POLYMERS cluster or other clusters or databases to create a multifile search environment for the purpose of trying out possible search strategies.

=> **INDEX POLYMERS**

```
INDEX 'APOLLIT, BABS, CAPLUS, CBNB, CIN, COMPENDEX, DISSABS,
EMA, IFIPAT, NTIS, PASCAL, PROMT, RAPRA, SCISEARCH,
TEXTILETECH, USPATFULL, USPATOLD, USPAT2, WPIDS, WPIFV,
WPINDEX, WSCA, WTEXTILES'
22 FILES IN THE FILE LIST IN STNINDEX
```

=> **S POLYURETHANE?**

• • •

L2 QUE POLYURETHANE?

=> **D RANK**

```
F1      227289   USPATFULL
F2      179086   CAPLUS
F3      152321   WPIDS
F4      152321   WPINDEX
F5      69717    IFIPAT
```

• • •

=> **FIL F1 F2 F4;S L2**

FILES 'USPATFULL, CAPLUS, WPINDEX' ENTERED AT ...
ALL COPYRIGHTS AND RESTRICTIONS APPLY. SEE HELP USAGETERMS
FOR DETAILS.

```
3 FILES IN THE FILE LIST
L3      227189   FILE USPATFULL
L4      179086   FILE CAPLUS
L5      152321   FILE WPINDEX
TOTAL FOR ALL FILES
L6      558596   L2
```

=> **D HIT 1 FROM EACH**

```
L6 ANSWER 1 OF 516000 USPATFULL on STN
SUMM U.S. Pat. No. 4,623,579 (Quon, Nov. 18, 1986),
incorporated herein by reference, discloses a decorative
composite article, which may be longitudinally slit to
form a yarn product, which has a combined phosphorescent
and fluorescent decorative appearance. The composite
article includes paired outer layers of a thermoplastic
resin between which is disposed a decorative layer
comprising a composition including a colorant component
having a phosphorescent colorant and a fluorescent
colorant, and a resin binder material. The fluorescent
colorant is present in an amount by weight that is up to
an amount equal to that of the phosphorescent colorant.
The present binder material may be selected from
polyester, polyurethane and acrylic polymers and
copolymers, with a mixture of butadiene-acrylonitrile
rubber and polyurethane composition being preferred.
```

(Continued on the next page)

The composite article is prepared by coating two resin films with the composition, followed by contacting the films with each other on their coated surfaces and applying heat and pressure to bond them together to form the decorative composite article.

L6 ANSWER 187749 OF 469415 CAPLUS COPYRIGHT 2009 ACS on

STN

AB This paper presents a method for sepg. viscothermal and scattering losses in ultrasonic characterization of porous media. This method is based on variations of the static pressure of the satg. fluid. Exptl. Results were already presented in previous papers and the losses sepn. was verified exptl. The aim of this paper is to present an analytic justification of this losses sepn. in the case of this exptl. method and to show that it is possible to est. acoustic parameters without the knowledge of scattering characteristics. The std. scattering length is used to renormalize speed and transmission through the porous medium, described as an equiv. fluid. Under certain assumptions corresponding to a weak scattering regime, it is shown how viscothermal and scattering losses can be sepd. easily without knowing scattering characteristics. Application of this model is presented in the case of weak scattering in a polyurethane foam and in the limit case of stronger scattering in a glass beads sample.

L6 ANSWER 337632 OF 469415 WPINDEX COPYRIGHT 2009 THOMSON REUTERS on STN

TI Fitness egg for performing finger exercises, is elliptical sphere filled with smooth, light density polyurethane rubber foam

TT TT: FIT EGG PERFORMANCE FINGER EXERCISE ELLIPSE SPHERE FILLED SMOOTH LIGHT DENSITY POLYURETHANE RUBBER FOAM

NOV NOVELTY - An elliptical sphere has a smooth surface and is filled with twenty to thirty five grams of strong light density polyurethane rubber foam. The elliptical sphere has a compatible shape of 100 mm length, 70mm width, 45 mm height, 130 mm radius.

**Polymer
databases with
CAS RNs**

The major polymer databases in addition to CA/CAPLUS that have CAS RN are:

- CBNB, CIN, PROMT
 - IFIPAT, IFICDB, IFIUDB
 - USPATFULL, USPAT2
-

**CAS RN
crossover**

Follow these steps for crossover of CAS RNs from REGISTRY to another database:

Step	Action
1	Create an answer set in REGISTRY.
2	Limit answer set to relevant CAS RNs. => S POLYAMIDE/PCT RAN=870967-04-7, L1 2511 POLYAMIDE/PCT
3	Enter target database(s). => FIL USPATALL FILES 'USPATFULL, USPAT2' ENTERED AT ... ALL COPYRIGHTS AND RESTRICTIONS APPLY. SEE HELP USAGETERMS FOR DETAILS. 2 FILES IN THE FILE LIST
4	Search the REGISTRY L-number. => S L1 AND 2009/PY TOTAL FOR ALL FILES L4 101 L1 AND 2009/PY

Note: Verify crossover fees prior to using CAS RN crossover.

**SELECT
NAME**

Searching for polymers in databases that do not contain CAS RN requires the use of polymer names. The SELECT NAME feature allows you to extract polymer names from a polymer search in REGISTRY and use them as search terms in other databases.

Step	Action
1	Create a polymer answer set in REGISTRY. => S ACRYLONITRILE (L) CHLOROETHYLENE AND PMS/CI AND 2/NC AND 1/CL L1 3 ACRYLONITRILE (L) CHLOROETHYLENE AND PMS/CI AND 2/NC AND 1/CL => D IN 1-3 L1 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN IN 2-Propenenitrile, polymer with 1-bromo-1- chloroethene (9CI) <i>(Continued on the next page)</i>

	<p>L1 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN</p> <p>IN 2-Propenenitrile, 2-methyl-, polymer with chloroethene (9CI)</p> <p>L1 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2009 ACS on STN</p> <p>IN 2-Propenenitrile, polymer with chloroethene (9CI)</p>
2	<p>Use SELECT NAME to create an E-number list.</p> <p>=> SEL NAME L1 3 E1 THROUGH E19 ASSIGNED</p>
3	<p>Use DISPLAY SEL to see the extracted names and E-numbers.</p> <p>=> D SEL</p> <p>E1 1 ACROPOR AN 200/BI E2 1 ACROPOR AN 450/BI E3 1 ACROPOR AN/BI E4 1 ACROPOR ANH/BI E5 1 ACROPOR WA/BI E6 1 ACROPOR/BI E7 1 ACROPORE/BI E8 1 ACRYLONITRILE-VINYL CHLORIDE COPOLYMER/BI E9 1 ACRYLONITRILE-VINYL CHLORIDE POLYMER/BI E10 1 AMICON XM 300/BI E11 1 DIAFLO XM 300/BI E12 1 DYNEL NYGL/BI E13 1 DYNEL/BI E14 1 KANEKALON/BI E15 1 METRICEL DM 450/BI E16 1 PM 6545/BI E17 1 SKHN 6/BI E18 1 VINYL CHLORIDE-ACRYLONITRILE COPOLYMER/BI E19 1 VINYON N/BI</p>
4	<p>Enter the target database(s).</p> <p>=> FIL APOLLIT COMPENDEX INPADOCDB INSPEC NTIS RAPRA SCISEARCH WPINDEX WTEXTILES FILES 'APOLLIT, COMPENDEX, INPADOCDB, INSPEC, NTIS, RAPRA, SCISEARCH, WPINDEX, WTEXTILES' ENTERED AT ... ALL COPYRIGHTS AND RESTRICTIONS APPLY. SEE HELP USAGETERMS FOR DETAILS. 9 FILES IN THE FILE LIST</p>
5	<p>Search the E-numbers.</p> <p>=> S E1-E19</p> <p>L3 46 FILE APOLLIT L4 14 FILE COMPENDEX L5 16 FILE INPADOC L6 6 FILE INSPEC L7 10 FILE NTIS L8 28 FILE RAPRA L9 7 FILE SCISEARCH</p> <p style="text-align: right;"><i>(Continued on the next page)</i></p>

```

L10          195 FILE WPINDEX
L11           33 FILE WTEXTILES
TOTAL FOR ALL FILES
L12          361 ("ACROPOR AN 200"/BI OR "ACROPOR AN
                450"/BI OR "ACROPOR AN"/BI OR
                "ACROPOR ANH"/BI OR "ACROPOR WA"/BI
                OR ACROPOR/BI OR ACROPORE/BI OR
                "ACRYLONITRILE-VINYL CHLORIDE
                COPOLYMER"/BI OR "ACRYLONITRILE-VINYL
                CHLORIDE POLYMER"/BI OR "AMICON XM
                300"/BI OR "DIAFLOXM 300"/BI OR
                "DYNEL NYGL"/BI OR DYNEL/BI OR
                KANEKALON/BI OR "METRICEL DM 450"/BI
                OR "PM 6545"/BI OR "SKHN 6"/BI OR
                "VINYLCHLORIDE-ACRYLONITRILE
                COPOLYMER"/BI OR "VINYON N"/BI)

=> D L12 HIT 1 FROM EACH
L12 ANSWER 1 OF 361 APOLLIT COPYRIGHT 2006 FIZ KA
on STN
TI Nanocomposites of vinyl chloride-
acrylonitrile copolymer and silica
• • •

```

ANALYZE NAME

ANALYZE NAME works similarly to SELECT NAME (above), but creates an L-number with the extracted terms instead of an E-number table.

```

=> S ACRYLONITRILE (L) CHLOROETHYLENE AND PMS/CI AND
    2/NC AND 1/CL
L1  3 ACRYLONITRILE (L) CHLOROETHYLENE AND PMS/CI
    AND 2/NC AND 1/CL

=> D IN 1-3
L1  ANSWER 1 OF 3 REGISTRY COPYRIGHT 2006 ACS on STN
IN  2-Propenenitrile, polymer with 1-bromo-1-chloroethene (9CI)
L1  ANSWER 2 OF 3 REGISTRY COPYRIGHT 2006 ACS on STN
IN  2-Propenenitrile, 2-methyl-, polymer with chloroethene (9CI)
L1  ANSWER 3 OF 3 REGISTRY COPYRIGHT 2006 ACS on STN
IN  2-Propenenitrile, polymer with chloroethene (9CI)
=> ANALYZE NAME L1 3
L2          ANALYZE L1 3 NAME :          19 TERMS

=> D L2
• • •
=> FIL POLYMERS -CASRNS -WPIDS
FILES 'APOLLIT, BABS, COMPENDEX, DISSABS, EMA, NTIS, PASCAL,
RAPRA, SCISEARCH, TEXTILETECH, WPIFV, WPINDEX, WSCA,
WTEXTILES' ENTERED AT ...
14 FILES IN THE FILE LIST

=> S L2/BI
TOTAL FOR ALL FILES
L3          362 L2/BI

```

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