

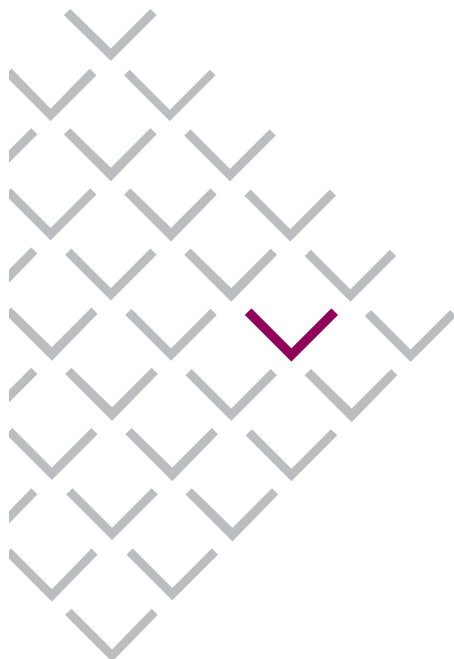


**Chemical Abstracts Service**  
provides access to STN International  
in North America

# STNNotes

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In response to customer requests for more detailed information on new and enhanced system features, we have created STNNotes. STNNotes give you the in-depth technical details you need for efficient use of STN. We hope you find this information useful. Please let us know how we can continue to improve in meeting your technical information needs.

## Enhanced Polymer Searching in CAS Files

**With the POLYLINK command, you can retrieve the CAS Registry Numbers<sup>®</sup> for the monomer-based and structural repeating unit representations for a given condensation polymer.**

Polymer searching in REGISTRY has been enhanced with:

- The POLYLINK command, which retrieves the monomer-based and structural repeating unit (SRU)-based CAS Registry Numbers<sup>®</sup> for a given condensation polymer or set of condensation polymers in a REGISTRY answer set
- Improved matching on SRUs in structure searches

In addition, starting in 2003, polymer index entries in CAPlus and CA are being enhanced by including multiple trade names and information about assumed monomers used to register a polymer.

### Polymer registration and indexing by CAS

A polymer is registered in REGISTRY based on the monomers that make the polymer, i.e., the polymer receives a monomer-based CAS Registry Number. This polymer may be made from many different monomers. It receives a different monomer-based CAS Registry Number for each set of monomers used.

In addition, for condensation polymers for which the structure of the unit that repeats down the polymer backbone can be identified unambiguously, another



CAS Registry Number is assigned based on the unambiguous SRU.

A condensation polymer is formed when monomer molecules combine, resulting in the loss of a small molecule such as water. Examples include polyesters, polyamides, polycarbonates, etc.

Documents are indexed using the monomer-based CAS Registry Number that has the particular monomers used in the reference or assumed by CAS document analysts. When there is an SRU-based CAS Registry Number for the polymer, the SRU-based CAS Registry Number may also be used in indexing. In some cases, depending on information available in the document, only an SRU-based or the monomer-based CAS Registry Number is indexed.

## POLYLINK – a command for linking polymers

With the POLYLINK command, you can retrieve the CAS Registry Numbers for the monomer-based and SRU representations for a given condensation polymer. POLYLINK may be used on:

- An individual CAS Registry Number
- An E-number containing a CAS Registry Number
- Any REGISTRY answer set
- Any ANALYZE list of CAS Registry Numbers

POLYLINK creates a new answer set containing the following answers:

- All of the CAS Registry Numbers in the original set
- All polymer CAS Registry Numbers that have been linked to the polymer CAS Registry Number in the original set

## Locate information on poly(tetramethylene carbonate).

```
=> FILE REGISTRY

=> S "POLY(TETRAMETHYLENE CARBONATE)"/CN
L1          1 "POLY(TETRAMETHYLENE CARBONATE)"/CN

=> POLYLINK L1
L2          16 POLYLINK L1

=> D SCAN

L2  16 ANSWERS  REGISTRY  COPYRIGHT 2004 ACS on STN
IN  Carbonochloridic acid, 1,4-butanediyl ester,
    polymer 1,4-butanediol (9CI)
MF  (C6 H8 Cl2 O4 . C4 H10 O2)x
CI  PMS

**RELATED POLYMERS AVAILABLE WITH POLYLINK**

      CM      1
      O         O
      ||        ||
Cl - C - O - (CH2)4 - O - C - Cl

      CM      2

      HO - (CH2)4 - OH

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

L2  16 ANSWERS  REGISTRY  COPYRIGHT 2004 ACS on STN
IN  Poly(oxy-carbonyloxy-1,4-butanediyl) (9CI)
MF  (C5 H8 O3)n
CI  PMS, COM

**RELATED POLYMERS AVAILABLE WITH POLYLINK**

      [
      O         O
      ||        ||
      O - C - O - (CH2)4 - O - C - O
      ]n

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

=> FILE CAPLUS

=> S L2
L3          94 L2

=> S L1
L4          78 L1
```

Enter **REGISTRY** and search the chemical name.

**POLYLINK** retrieves **15 additional CAS Registry Numbers** for the polymer in **L1**.

**Examples of additional CAS Registry Numbers** retrieved via **POLYLINK** are shown in **D SCAN** of the answer set.

**Sixteen additional answers** are retrieved from **CAplus** by using the **CAS Registry Numbers** in the **POLYLINK** answer set (**L2**).

Note that POLYLINK functions the same way regardless of whether the starting set contains one or more of the monomer-based or SRU-based CAS Registry Numbers.

To remind you that additional relevant CAS Registry Numbers might be available for a polymer, the message **\*\*RELATED POLYMERS AVAILABLE WITH POLYLINK\*\*** appears along with structure displays on STN. In addition, the term **RELATED POLYMERS/FA** is posted to each CAS Registry Number that has at least one additional polymer CAS Registry Number linked to it and can be used to isolate polymer CAS Registry Numbers in an answer set that have one or more polymer CAS Registry Numbers linked to it.

## Cost

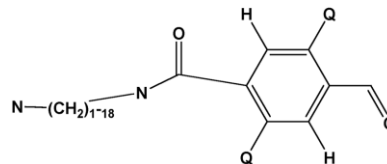
There is a flat charge for every use of the POLYLINK command. Enter HELP COST in REGISTRY or ZREGISTRY for cost information.

## Improved SRU retrieval

CAS has improved searching polymers on the basis of SRUs, so that you no longer need to know the CAS nomenclature rules for ordering atoms in SRUs.

You can construct a comprehensive SRU-based search query by simply creating and searching any structure fragment of the polymer backbone. The structure search process automatically matches your query structure with the appropriate SRU representations in the file.

**Locate information on polymers containing the following structure fragment in the polymer backbone.**



=> **FILE REGISTRY**

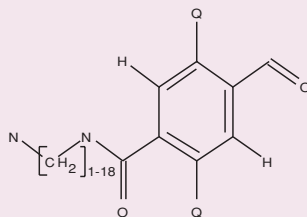
=>  
Uploading C:\Program  
Files\Stnexp\Queries\polyamide.str

L1 STRUCTURE UPLOADED

=> **D L1**

L1 HAS NO ANSWERS

L1 STR



=> **S L1 SSS FULL**

FULL SEARCH INITIATED 12:06:28 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 52962 TO ITERATE

100.0% PROCESSED 52962 ITERATIONS 31 ANSWERS  
SEARCH TIME: 00.00.13

L2 31 SEA SSS FUL L1

=> **S L2 AND PMS/CI**

929249 PMS/CI

L3 12 L2 AND PMS/CI

=> **D SCAN**

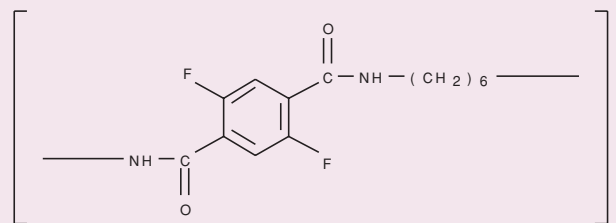
L3 12 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN

IN Poly[iminocarbonyl(2,5-difluoro-1,4-

phenylene)carbonylimino-1,6-hexanediyl] (9CI)

MF (C14 H16 F2 N2 O2)n

CI **PMS**

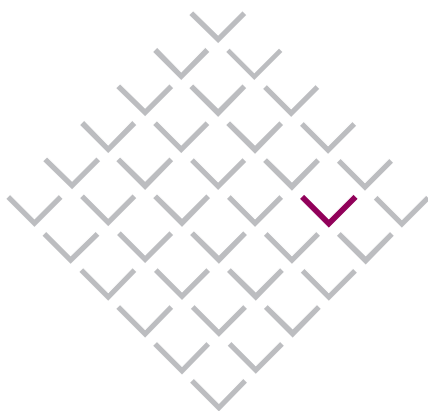


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

**Enter REGISTRY and search the uploaded structure.**

**Combine the structure search results with PMS/CI to limit answers to polymers.**

**Additional SRUs with backbone structures such as the one shown are retrieved as a result of the improved SRU matching process. Note that this answer does not have a N atom following the repeating group. You must "wrap" to the beginning of the SRU representation to pick up the second nitrogen atom.**



## Enhanced polymer indexing

Starting in 2003, polymer index entries in CAplus and CA are being enhanced by:

- Including multiple trade names for the same polymer when the trade names are provided in the original document
- Providing information in a text-modifying phrase that assumed, rather than actual, monomers specified in the document were used to register a polymer

### An example of an index entry with multiple trade names.

IT 9002-88-4, Polyethylene  
 RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)  
 (**Hiwax 110P, Hizex Million 340M**; polyolefin-based agricultural mulching films with good air and moisture permeability)

### An example of an index entry for a polymer registered using assumed monomers.

IT 26062-94-2, 1,4-Butanediol-terephthalic acid copolymer  
 RL: PEP (Physical, engineering or chemical process); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)  
 (**assumed monomers**, closed-cell foams; polyester core materials and structural sandwich composites thereof)

## For more information

Enter HELP POLYLINK at an arrow prompt for online information about the POLYLINK command.

For Web access to this STNote, visit:

[www.cas.org/ONLINE/STN/STNOTES/stnotescover.html](http://www.cas.org/ONLINE/STN/STNOTES/stnotescover.html)