Session Agenda

- Polymer definition
- STN files with polymer information
- Polymers in CAS files
- Searching polymers in Registry
- Searching polymers in CAplus
- Polymer property information
Polymers are large chemicals made up of smaller units (monomers) combined together to form chains.

Polymers may be natural or synthetic.

Plastics, rubbers, protein/nucleotide sequences, fibers, and adhesives are all polymers.
Polymers on STN

- Scientific & Technical Information Network
- More than 200 databases in all areas
- Browser-based access available at http://stnweb.cas.org:
STN Files on Polymers

♦ Chemical & Material Files:
  • CAplus, DKILIT, EMA, RAPRA, TEXTILETECH, WTEXTILES

♦ Substance Files
  • CHEMLIST, PDLCOM, PLASPEC, REGISTRY

♦ Property Files
  • ASMDATA, CAplus, DKILIT, PDLCOM, PLASPEC
STN Files on Polymers

♦ Business & News Files
  • CBNB, CEN, CIN, PLASNEWS, PROMT

♦ Patent Files
  • CAplus, IFIPAT, USPATFULL, USPAT2, WPIDS, WPINDEX
Polymers in CAS Files

- World’s largest and most current source of polymer information
- Indexing of synthetic polymers is usually based on monomers used to prepare them
- Supplemental indexing provided selectively for structure of the final polymer
Types of polymers

♦ Addition (vinyl) polymerization

\[ n \text{ CH}_2=\text{CHCl} \rightarrow -(\text{CH}_2-\text{CH})_n- \]

- where \( n > 10 \) or an unspecified number
- monomer-based Registry Number only
Types of polymers

♦ Condensation polymerization

- monomer-based Registry Number
- supplemental Registry Number for structural repeating unit (SRU) if monomers are symmetrical
Polymers in Registry

- The Registry file contains more than 928,038 polymeric substances (6/6/02)
- Registry is updated daily with new polymer entries
- Each polymer record is assigned an unique CAS Registry Number (RN)
- The RN can be used in bibliographic files to find corresponding references to the substance
Factors that DO NOT affect polymer registration:

- Molecular weight
- Monomer ratio in addition polymers
  - e.g., 60:40 and 90:10 ethylene-vinyl chloride copolymers have the same Registry Number
- Head-to-head versus head-to-tail arrangements
Polymers in Registry

Factors that DO affect polymer registration:

♦ Tacticity (stereochemistry)
  • atactic polypropylene (NS) 9003-07-0
  • isotactic polypropylene 25085-53-4
  • syndiotactic polypropylene 26063-22-9

♦ Presence of end-groups (SRU only)

♦ Block, graft, alternating polymer forms
  • only since 1987
Registry Sample Record

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 9003-53-6 REGISTRY
CN Benzene, ethenyl-, homopolymer (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN 105E
CN 138F

Other Names includes trade name designations and common names

o o o
CN Styrene homopolymer
ADDITIONAL NAMES NOT AVAILABLE IN THIS FORMAT
- Use FCN, FIDE, or ALL for DISPLAY
MF (C8 H8)x
CI PMS, COM
PCT Polystyrene
Registry Record Continued

LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, ASMDATA*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEM CATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DDFU, DETHERM*, DIOGENES, DRUGU, EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MSDS-OHS, NIOSHTIC, PDLCOM*, PHARMASEARCH, PIRA, PLASPEC*, PROMT, RTECS*, SPECINFO, TOX CENTER, TULSA, ULIDAT, USPAT2, USPATFULL, VTB
(*File contains numerically searchable property data)

Other Sources: DSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

The Registry Number Locator field lists STN files that can be searched for information about the polymer
Registry Record Continued

CM    1

CRN   100-42-5
CMF   C8  H8

H2C=CH-Ph

83466 REFERENCES IN FILE CAPLUS (1967 TO DATE)
Finding RN’s for Polymers
### Registry Search Fields

<table>
<thead>
<tr>
<th>Search Field</th>
<th>Field Code</th>
<th>Example</th>
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<tbody>
<tr>
<td>CAS Registry Number</td>
<td>/RN</td>
<td>S 29035-74-3</td>
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<tr>
<td>(or none)</td>
<td>/CRN</td>
<td>S 110-63-4/CRN</td>
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<td>Component Registry Number</td>
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<tr>
<td>Chemical Name</td>
<td>/CN</td>
<td>S POLYSTYRENE/CN</td>
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<tr>
<td>Molecular Formula</td>
<td>/MF</td>
<td>S &quot;(C8H8)X&quot;/MF</td>
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<tr>
<td>Number of Components</td>
<td>/NC</td>
<td>S L1 AND 2/NC</td>
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<tr>
<td>Polymer Class Term</td>
<td>/PCT</td>
<td>S POLYSTYRENE/PCT</td>
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### Finding Polymers by Name

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<th>E</th>
<th>VINYL CHLORIDE POLYMER/CN</th>
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<tbody>
<tr>
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<td>VINYL CHLORIDE OCTAMER/CN</td>
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<tr>
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<td>VINYL CHLORIDE PENTAMER/CN</td>
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<tr>
<td>E3</td>
<td>1</td>
<td>--&gt; VINYL CHLORIDE POLYMER/CN</td>
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<td>VINYL CHLORIDE RADICAL CATION/CN</td>
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<td>E5</td>
<td>1</td>
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<td>VINYL CHLORIDE TETRAMER/CN</td>
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<td>VINYL CHLORIDE TRIMER/CN</td>
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O O O

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<th>E3</th>
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<tbody>
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<td>&quot;VINYL CHLORIDE POLYMER&quot;/CN</td>
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</table>
Finding Polymers by Name

=> D

L1   ANSWER 1 OF 1  REGISTRY COPYRIGHT 2002 ACS
RN   9002-86-2  REGISTRY
CN   Ethene, chloro-, homopolymer (9CI)
     (CA INDEX NAME)
OTHER NAMES:
CN   1000Z
CN   101EP
CN   1032X
O O O
CN   Amerace A 30
CN   Vinyl chloride polymer
O O O
Finding Polymers by CRN

♦ **Step 1** Find the RN for each monomer.
♦ **Step 2** Search RN in the Component Registry Number (/CRN) field.
♦ **Step 3** Combine using AND operator.
♦ **Step 4** Limit by Number of Components (/NC) field.
Finding Polymers by CRN

=> S L3 AND 2/NC
   2620877 2/NC
L4  5 L3 AND 2/NC

=> D SCAN
L4  5 ANSWERS  REGISTRY  COPYRIGHT 2002 ACS
IN  1,4-Benzenedicarboxylic acid, polymer with 1,2-ethanediol(9Cl)
MF  (C8 H6 O4 . C2 H6 O2)x
CI  PMS, COM

   CM  1

   HO—CH2—CH2—OH

   CM  2

   HO2C

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):END
Polymer class terms (PCT's) describe broad classes of polymers. The current REGISTRY PCT's are:

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

=> FIL REG

=> S FLUOROPOLYMER/PCT
L1 8566 FLUOROPOLYMER/PCT

=> FIL HCAPLUS

=> S L1
L2 61224 L1
## Polymer Terms in HCAplus

### FLUOROPOLYMERS/CT

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<th>TERM</th>
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<td>FLUOROPOLYMER-URETHANE/CT</td>
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<tr>
<td>E2</td>
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<tr>
<td>E3</td>
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<td>245</td>
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<tr>
<td>E4</td>
<td>0</td>
<td>5</td>
<td>FLUOROPOLYMERS (L)</td>
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### E3+NT1/CT

| E1 | 42833 | FLUOROPOLYMERS/CT |

**NOTE** Polymers having a C-F bond in the repeating portion of the chain are indexed here.

| E2 | 0     | NT1 Chlorotrifluoroethylene-ethylene copolymer/CT |
| E3 | 0     | NT1 Chlorotrifluoroethylene-vinylidene fluoride copolymer/CT |
| E4 | 0     | NT1 Ethylene-tetrafluoroethylene copolymer/CT      |
| E5 | 1746  | **NT1 Fluoro rubber/CT                           |

O O O
Polymer Terms in HCAplus

=> S E3+ALL
L3  206035  FLUOROPOLYMERS+ALL/CT  (245 TERMS)

=> S L2 OR L3
L4  208494  L2 OR L3

=> S L4(L) ANTIFRICTION COATING#
L5  83  L4(L) ANTIFRICTION COATING#
Fluoro rubber
(chlorotrifluoroethylene-vinylidene fluoride, SKF 32; antifriction coatings from fluoro rubber vulcanized under laser radiation)

9010-75-7, Chlorotrifluoroethylene-vinylidene fluoride copolymer
(rubber; antifriction coatings from fluoro rubber vulcanized under laser radiation)
## Finding Polymer Properties

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<th>Property</th>
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<td>Mechanical properties/CT</td>
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<td>Toughness/CT</td>
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********** END***
Finding Polymer Properties

=> INDEX PLASDATA
INDEX 'ASMDATA, PDLCOM, PLASPEC' ENTERED
3 FILES IN THE FILE LIST IN STNINDEX

=> S NOVADOWNL
0 FILES HAVE ONE OR MORE ANSWERS, 3 FILES SEARCHED IN STNINDEX
L1 QUE NOVADOWNL

=> FIL REG

=> S L1

L2 1 NOVADOWNL

=> D
L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 26062-94-2 REGISTRY
CN 1,4-Benzenedicarboxylic acid, polymer with
1,4-butanediol (9CI) (CA INDEX NAME)
### Finding Polymer Properties

```plaintext
=> SEL CHEM
E1 THROUGH E25 ASSIGNED

=> DIS SEL

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<tr>
<th>E</th>
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<td>E3</td>
<td>1</td>
<td>BUTYLENE GLYCOL-TEREPHTHALIC ACID POLYMER/BI</td>
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<tr>
<td>E4</td>
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<td>NOVADOWL/BI</td>
</tr>
<tr>
<td>E25</td>
<td>1</td>
<td>26062-94-2/BI</td>
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</table>

=> FIL PLASPEC

=> S E1-E25
```
Material Class: Thermoplastic
Family Name: Polybutylene terephthalate
Trade Name and Grade: Crastin S660FR
CAS Registry Number: 24968-12-5 (Polybutylene terephthalate), 26062-94-2 (Polybutylene terephthalate)
Resin Form: pellets
Supplier: DuPont Engineering Polymers
Application: Electrical
Features: Flame retardant
Finding Polymer Properties

Processing/Physical Characteristics

Process Type: Injection molding
Recommended Melt Temperature: 464 - 500 deg F
Density: 1.45 g/cm**3 at ambient temperature
Shrinkage, Mold: 1.8 in/in in machine direction
                      2.2 in/in in transverse direction
Water Absorption, 24 Hour: 0.06%

Mechanical Properties

Elongation at Break: 10%
Flexural Yield Strength: 1.17E+04 psi
Compressive Ultimate Strength: 1.06E+04 psi
Modulus of Elasticity
   Tensile: 4.3E+05 psi
   Flexural: 3.9E+05 psi
Finding Polymer Properties

Hardness

Rockwell: R116
Izod Impact Energy, Normalized: 0.8 ft*lbf/in for 0.125 in wide specimen

Thermal Properties

Melting Point: 437 deg F
Linear Expansion Coefficient: 7E-05 in/in*deg F

Electrical Properties

Dielectric Strength
Short Time: 400 V/mil
Dielectric Constant: 3 at 60 Hz
Volume Resistivity: 1E+16 ohm*cm
Surface Resistivity: 5E+14 ohm