

Multiple-Level Polymer Registration in the DuPont SCION Database

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The Chemical Abstracts Service Registry System (CASRS) has a relatively unknown but very useful feature; with the exception of one situation, it has the capability of multiple-level source-based polymer registration, i.e., it will register a source-based polymer within a source-based polymer. The CASRS registers macromonomers in File Registry as single-component substances. In contrast, macromonomers registered in the DuPont SCION proprietary database by the CASRS are represented as *multicomponent* substances. Single-level CASRS registration of comb polymers in SCION currently results in loss of identity of macromonomers as searchable components. Multilevel source-based registration provides a way to register multicomponent macromonomers as components of comb polymers so that their registration numbers become part of comb polymer structure records.

1. INTRODUCTION

SCION is a proprietary database managed by Chemical Abstracts Service (CAS) exclusively for DuPont. Registration of polymers is executed manually for DuPont by CAS keyboarding personnel.

In a manner similar to the function of CAS's File Registry, SCION chemical file records for chemical substances are stored via the CAS Registry System (CASRS) and searched via Messenger software. The chemical file of the SCION database, described in an earlier publication,¹ follows CAS structure conventions except in the polymer field, where appreciable differences exist. Among these major differences are conventions for macromonomers and comb polymers therefrom.

In SCION, macromonomers are registered as multiple-component source-based polymers; see Chart 1.

The class identifier (CI) in Chart 1 is PMS,COM; this indicates that the records are both polymers (PMS) in their own right and components (COM) of other multicomponent substances, e.g., comb polymers. An important feature of both the CAS File Registry and the chemical file of the SCION database is that searches of CAS RNs (in File Registry) or CNUMs (in SCION) of components of polymers with the /CRN suffix ("Component Registry Number" field qualifier) retrieve all macromonomers and comb polymers containing them.

Thus, in File Registry the search strategy

⇒ S 26915-72-0/CRN AND PMS/CI

where 26915-72-0 is the RN of a macromonomer, retrieves all comb polymers containing it.

In the SCION chemical file the search strategy

⇒ S (100A AND 200B AND 300C)/CRN AND PMS/CI

retrieves both the macromonomer of structure 1.1 and any comb polymers containing these components. However, for

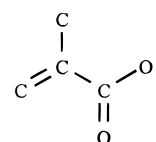
Chart 1. SCION Record for "Methoxy Polyethylene Glycol Methacrylate" Macromonomer^a

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CNUM: 400D
DUP: POLY-OXYETHYLENE, END GROUP METHACRYLOYLOXY, END
GROUP METHOXY
:
MF: (C4 H5 O2 . (C2 H4 O)n . C H3 O)x
CI: PMS, COM
STE: 8:DP,EGPCC
```

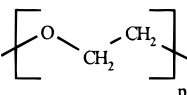
```
COM 1
CNUM 100A
MF C H3 O
CI COM
STE 8:DP,FRA
```

.Ole

```
COM 2
CNUM 200B
MF C4 H5 O2
CI COM
STE 8:DP,FRA
```



```
COM 3
CNUM 300C
MF (C2 H4 O)n
CI PMS, COM
```



^a (1) In this paper, colons indicate deleted sections of records not pertinent to the discussion; (2) C-Numbers [CNUMs; SCION equivalent of CAS Registry Numbers (RN)] are disguised for security reasons; (3) the reason why the polymerizable end group in the SCION record is METHACRYLOYLOXY, vice METHACRYLOYL, is to preserve the entire functional group; this is explained fully elsewhere;¹ (4) the text descriptor 8:DP,EGPCC is explained in section 3.

reasons that are discussed in this paper, the search strategy

⇒ S 400D/CRN AND PMS/CI

where 400D is the CNUM for the macromonomer in Chart 1, does *not* currently retrieve comb polymers containing this macromonomer.

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The multiple-component method for macromonomer registration used in SCION has one major advantage and two disadvantages, one minor and one more serious. The major advantage is that end groups can be searched as components of macromonomers because they have individual structures and CNUMs. Thus, the question "Find structures of all macromonomers that contain the methacryloyloxy end group or comb polymers containing them" is answered by the *precise* search strategy

⇒ S 200B/CRN AND PMS/CI

where 200B is the CNUM for the methacryloyloxy fragment. Fragments such as these are theoretical polymer components, with CNUMs, that are created expressly to facilitate searching; they are not real fragments or free radicals.²

In File Registry, this question can be answered only by use of a combination of controlled terms and free-text terms in a more complex search. Searchers have to be knowledgeable about nomenclature; they must also remember that the group may be at the α end or the ω end of a polymer. A sample search in File Registry with the strategy

⇒ S PMS/CI AND 2-METHYL-1-OXO-2-PROPENYL*

*CA 9th Collective Index equivalent of "methacryloyl"

retrieved about 22 000 answers. Modifying the strategy to

⇒ S PMS/CI AND

2-METHYL-1-OXO-2-PROPENYL AND GRAFT

retrieved about 1500 answers (CAS classifies comb polymers as graft polymers).

The problem with free-text searching, of course, is that the computer selects every occurrence of the chosen words or phrases, regardless of whether it is an intellectual answer. This sample search indicates that less than 7% of the occurrences of the expression 2-METHYL-1-OXO-2-PROPENYL are associated with graft or comb polymers; without screening the answers, it is still unknown whether all 1500 answers are pertinent. Clearly, this approach does *not* give an intellectually "clean" answer.

CAS registration of comb copolymers with the term "graft" as an integral part of the Registry record began with the 12th Collective Index (1987). Earlier records are incomplete in their recognition of comb polymers as such; some have the word "graft" somewhere in the text but are not classified as graft polymers, while others have no recognition at all. Earlier records are therefore not retrieved by this strategy. Additionally, CAS does not distinguish between graft and comb polymers, and (as stated above) classifies comb polymers as graft polymers, which adds to the uncertainty of the answers retrieved.

The minor disadvantage of the SCION multiple-component method is that the number-of-components operator, the so-called "/NC field qualifier", is usually different when macromonomers are being searched in the SCION chemical file versus a File Registry search. Thus, File Registry macromonomers may be retrieved by use of Boolean logic that uses 1/NC (or NC = 1), whereas SCION chemical file macromonomers may be retrieved by use of 2/NC (or NC = 2) (for those with one end indexed as part of the structure record) and 3/NC (or NC = 3) (for those with both ends

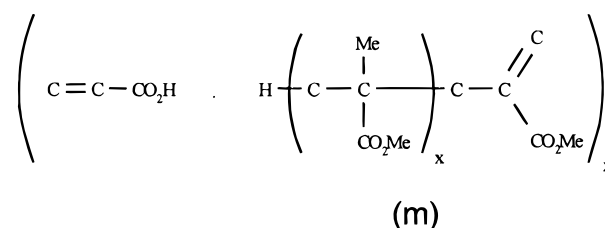
indexed as part of the structure record). These differences naturally also affect retrieval of comb polymers containing such macromonomers.

The second (more serious) disadvantage is the inability to search easily for macromonomers as components of comb polymers; this is described in the next section.

2. CURRENT REGISTRATION METHOD IN SCION CHEMICAL FILE

Because of the rarity in File Registry of polymers of the type $(A(B)_x)_x$, where A and B are *source-based* monomers, until very recently the fact that the CASRS can register an expression containing a source-based polymer within a source-based polymer was unknown to both of us; thus, a theoretical structure such as that shown in example 2.1 below was believed by us to be unregistrable.

Example 2.1. "Polymer within a polymer" (source-based registration); comb polymer from poly(methyl methacrylate) macromonomer and acrylic acid

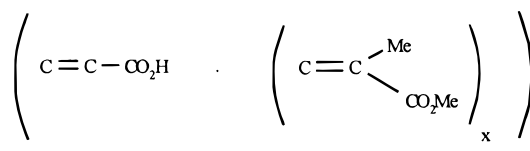


Component m in this example is a pictorial representation of the poly(methyl methacrylate) macromonomer with a hydro end group and a 2-(methoxycarbonyl)allyl end group. Although the diagram shows it, precise head-to-head or head-to-tail linking within the polymer chain is *not* implied; this is merely a way of indicating the concept $\text{H}(\text{C}_5\text{H}_8\text{O}_2)_x\text{C}_5\text{H}_7\text{O}_2$. Use of subscript x , vice subscript n , is intended to convey the concept that poly(methyl methacrylate) is *source-based* (see point 1).

Point 1. The use of subscript x within subscript x is used throughout this paper to convey the idea of a source-based polymer within a source-based polymer.

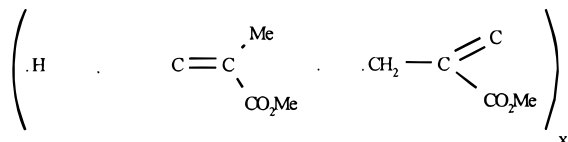
Such a structure is registrable by the CASRS, but it is CAS policy not to register structures such as that shown in example 2.1. Instead, this polymer would be registered in File Registry as shown in example 2.2;³ regrettably, end group data are omitted (this is discussed in more detail in section 3 below).

Example 2.2. CAS source-based representation of comb polymer from poly(methyl methacrylate) macromonomer and acrylic acid



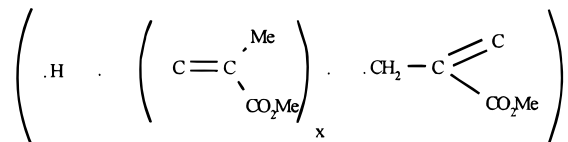
Macromonomers with a polymerizable end group such as $\text{H}(\text{C}_5\text{H}_8\text{O}_2)_x\text{CH}_2\text{C}(\text{CO}_2\text{Me})=\text{CH}_2$ derived from poly(methyl methacrylate) are registered in SCION as three separate-moieties primarily to register end groups as individual entities with searchable CNUMs; see example 2.3. Compromises in the structural representation of comb polymers in SCION were therefore made because they were believed by us to be necessary.

Example 2.3. Source-based representation in SCION of the poly(methyl methacrylate) macromonomer (current record)



The end groups are registered as fragments. The structure of example 2.3 is, in itself, an inexactitude, because in reality only the methyl methacrylate is the repeating part; the ideal representation is as shown in example 2.4.

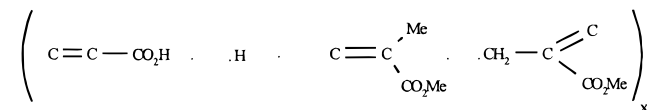
Example 2.4. Ideal source-based representation of the poly(methyl methacrylate) macromonomer



Such a structure is registrable, but it would not receive the overall designation of PMS/CI (polymers/class identifier), i.e., it would be perceived not as a polymer but *containing* a polymer. The representation shown as example 2.3 is an acceptable compromise.

Registration in SCION of comb polymers such as that formed from acrylic acid and the poly(methyl methacrylate) macromonomer (shown in its ideal form as example 2.1) is currently a single-level expression in which all four moieties are registered, see example 2.5.

Example 2.5. Current single-level, source-based registration of the comb polymer from acrylic acid and the poly(methyl methacrylate) macromonomer



Component CNUMs: 456D 123A 345C
Macromonomer CNUM: ← 234B →

In polymers such as that shown as example 2.5, each component has a registration number (CNUM); the CNUM for acrylic acid is not shown because it is not pertinent to the discussion. In a manner similar to that used in CAS's File Registry, the CNUM of a monomer [or structural repeating unit (SRU)] can be used to find polymers that contain that monomer or SRU. Thus, if 123A is the CNUM of monomeric methyl methacrylate, the search strategy

⇒ S 123A/CRN AND PMS/CI

locates all polymers containing methyl methacrylate as a component.

However, the CNUM of this poly(methyl methacrylate) macromonomer, assume 234B for discussion purposes, is *not, per se*, a component of comb polymers such as that shown in example 2.5. It is therefore currently impossible to obtain a direct answer to the question "How many comb polymers contain this specific poly(methyl methacrylate) macromonomer?" by the simple search strategy

⇒ S 234B/CRN AND PMS/CI

This search currently results in zero answers. To answer the question, it is necessary to search for both the macromonomer and comb polymers containing it with the search strategy

⇒ S (123A AND 345C AND 456D)/CRN AND PMS/CI

wherein 345C and 456D are CNUMs for the 2-(methoxycarbonyl)allyl and hydro fragments of the complete macromonomer, respectively; see example 2.5.

This retrieves both this specific macromonomer and comb polymers containing it. The macromonomer itself can be excluded from the search by modifying the strategy to

⇒ S (123A AND 345C AND 456D)/CRN AND PMS/CI AND
POLY-COMB-OR-GRAFT/CT (see point 2)

Point 2. Comb and graft polymers are perceived intellectually by DuPont's Corporate Information Systems polymer registration personnel to be appreciably different, and they are registered by different techniques;¹ however, because comb polymers are frequently referred to as graft polymers, the controlled term POLY-COMB-OR-GRAFT is applied to all comb and graft polymers.

This strategy works, but it is esthetically unsatisfactory because it does not parallel CAS's technique of searching for comb polymers containing macromonomers by searching in File Registry with the CAS Registry Number of the macromonomer followed by the /CRN field qualifier. Chemists typically perceive macromonomers as *single* substances, rather than two- or three-component substances, and the current inability to search for them in SCION as single substances with a single CNUM thus leads to considerable frustration for searchers.

Resolution of this problem is presented in the next section.

3. SOLUTION TO THE PROBLEM

Since the introduction of so-called "Registry III" in the early 1970s,³ the CASRS has had an obscure but very useful feature, multilevel polymer registration capability; this is the ability to register expressions containing a source-based polymer (as opposed to a structure-based polymer, i.e., an SRU) within a source-based polymer. The feature is not well-known, and one of us (E.S.W.) learned about it purely by chance. CAS personnel do not teach it in their polymer-searching courses, and it is discussed in neither of two important CAS publications on polymer registration policy and searching techniques.^{4,5} This feature is used very little in CAS polymer registration, which probably accounts for its obscurity.

In File Registry a macromonomer structure comprising an addition polymer is registered as (A)_x, where A is a monomer;³ see example 3.1.

Example 3.1. CAS structure for a polymer containing an addition-polymer macromonomer

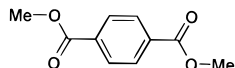
In polymers of this type the end groups are currently omitted from the structure; thus, there is no indication of whether this is, for example, a linear, single-strand polyester (see example 3.2a), a comb polymer (see example 3.2b), or some other type. Naturally, CAS is aware of this deficiency; its correction is planned as part of a future Registry File enhancement.³

RN 66167-61-1 REGISTRY
 CN 1,4-Benzenedicarboxylic acid, dimethyl ester, polymer with ethene homopolymer (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Ethene, homopolymer, polymer with dimethyl 1,4-benzenedicarboxylate (9CI)
 MF (C10 H10 O4 . (C2 H4)x)x
 CI PMS
 PCT Polyolefin, Polyether
 LC STN Files: CA, CAPLUS, TOXLIT

CM 1

CRN 120-61-6

CMF C10 H10 O4



CM 2

CRN 9002-88-4

CMF (C2 H4)x

CCI PMS

CM 3

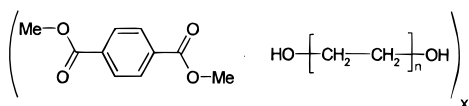
CRN 74-85-1

CMF C2 H4

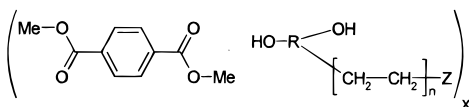
H₂C=CH₂

Example 3.2. Possible interpretations of the polymer shown as example 3.1

3.2a. Linear, single-strand polyester from α,ω -dihydroxy-ended poly(ethylene)



3.2b. Comb polymer from α,α -dihydroxy-ended poly(ethylene) (R = junction point; Z = nonpolymerizable end group)



In contrast, a macromonomer structure comprising a condensation polymer is registered as EG(A)_nEG (where A is an SRU and EG is an end group). The atoms from both end groups are added together to form a nonpolymeric part of the molecular formula; see example 3.3. This type of macromonomer is much more frequently encountered.

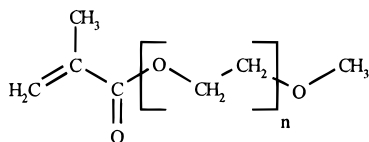
3.3. CAS structure for "methoxy polyethylene glycol methacrylate" macromonomer

RN 26915-72-0 REGISTRY
 CN Poly(oxy-1,2-ethanediyl), α -(2-methyl-1-oxo-2-propenyl)- ω -methoxy- (9CI) (CA INDEX NAME)

MF (C2 H4 O)_n C5 H8 O2

CI PMS, COM

PCT Polyether

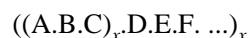


With the realization (by E.S.W.) that adaptation of the CASRS *source-based* multilevel polymer registration technique could be used to solve the problem described in section 2, a program to reregister comb polymers in SCION was initiated; the modified format ensures that the CASRS includes CNUMs for macromonomers as descriptors (see

point 3) of comb polymers. This, in turn, ensures that they are searchable with the /CRN field qualifier to retrieve comb polymers of which they are a component.

Point 3. In the SCION chemical file, CNUMs of components of polymers are called descriptors. Thus, the CNUM of ethylene is a descriptor to all polymers containing ethylene as a component.

The revised comb polymer registration technique is as follows: (1) parenthesize the components that comprise the macromonomer, (2) place a subscript x outside the right-hand parenthesis, (3) add the rest of the comonomers to the expression, and (4) parenthesize the whole expression and again add a subscript x outside the right-hand parenthesis. Dots are placed between the components of the expression. Thus, for a comb polymer derived from a macromonomer (A.B.C)_x (wherein B is a monomer and A and C are polymer fragments) that is copolymerized with other comonomers D, E, F, etc., the expression is:



Note: in structural representations, CAS uses parentheses to indicate polymers (expressions with a subscript x) and brackets to indicate SRUs (expressions with a subscript n); thus, in this and other similar expressions in this paper denoting a polymer within a polymer, multiple sets of parentheses are correct.

In addition to the macromonomer (A.B.C)_x, at least one other monomer must be present; thus, registration of ((A.B.-C)_x)_x fails. Section 4 discusses resolution of this problem in SCION.

The physical layout of the display of a restructured comb polymer conveys important information about the multilevel nature of the stored record; thus, in Chart 2, the second component (COM 2), the macromonomer, itself contains three more components (COM 3, COM 4, and COM 5), and these are indented in the display.

Key points of the reregistered comb polymer are as follows: First, the macromonomer (CNUM 8910H) is a component of the comb polymer (CNUM 91011J), i.e., the search strategy S 8910H/CRN AND PMS/CI retrieves the comb polymer containing the macromonomer. Second, the fluoro fragment, the C₆H₉O₂ fragment, and tetrafluoroethylene (CNUMs 567E, 678F, and 789G, respectively) are components of the macromonomer (CNUM 8910H) and also of the comb polymer (CNUM 91011J), i.e., the search strategy S (567E AND 678F AND 789G)/CRN AND PMS/CI retrieves both the macromonomer (CNUM 8910H) and the comb polymer.

Chart 2 also shows application, for identification purposes, of special text descriptors to the macromonomer and to the comb polymer.

At the highest (comb polymer) level, the descriptor is 8:DP,COMB. This has intelligence built into it: "8:" signifies a CAS class 8 substance (which includes polymers); "DP" signifies DuPont (code assigned by CAS to DuPont); and "COMB" signifies a comb polymer. Descriptors such as these are needed to ensure, for example, that two polymers with the same components but different configurations are recognized by the CASRS as unique. Thus, block polymers such as (A.B)_x are registered with the descriptor 8:DP,BLO to distinguish them from the corresponding random or statistical polymers (A.B)_x.

Chart 2. Comb Polymer from Methyl Methacrylate (CNUM 123A) and the Macromonomer F(C₂F₄)_xCH₂CH₂CH₂OCOCH=CH₂ (CNUM 8910H)^a

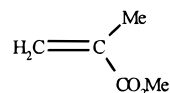
CNUM:91011J

MF: ((C6 H9 O2 . C2 F4 . F)x . C5 H8 O2)x (see note below structure part of record)

CI: PMS

STE: 8:DP,COMB

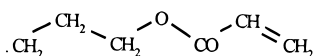
COM 1
CNUM 123A
MF C5 H8 O2
CI COM



COM 2
CNUM 8910H
MF (C6 H9 O2 . C2 F4 . F)x
CI PMS, COM
STE 8:DP,EGPCC

COM 3
CNUM 567E
MF F
CI COM
STE 8:DP,FRA
.F

COM 4
CNUM 678F
MF C6 H9 O2
CI COM
STE 8:DP,FRA



COM 5
CNUM 789G
MF C2 F4
CI COM
F2C=CF2

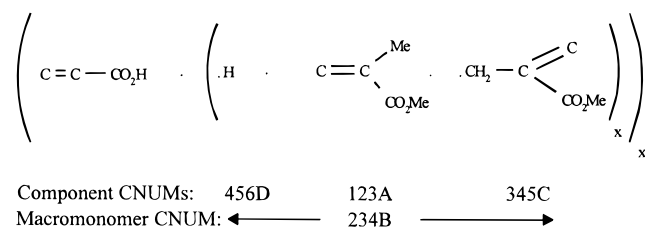
^aBecause the CASRS will not accept brackets in substance names in SCION, multiple parentheses are used in place of the customary combination of parentheses and brackets; online displays also show multiple parentheses, vice a combination of parentheses and brackets.

At the intermediate level, the descriptor for the macromonomer is 8:DP,EGPCC. EGPCC, the abbreviation for "end group polymerizable CC", denotes a macromonomer with a polymerizable carbon-carbon multiple bond.

At the lowest level, the descriptors used are the ones normally associated with nonpolymeric substances; the one shown, 8:DP,FRA, is used for polymer fragments such as fluoro and 3-(methacryloyloxy)propyl. Other typical ones (not exemplified in this paper) denote attributes such as absolute stereoisomerism (e.g., 1:R) and geometrical isomerism (e.g., 2:Z); these are the standard ones used by CAS, and they have the same meanings.

Thus, the comb polymer currently registered in the SCION chemical file as shown in example 2.5 will be reregistered as shown in example 3.4. The new expression to be keyed contains a polymer within a polymer.

Example 3.4. Revised source-based representation of a polymer within a polymer; comb polymer from poly(methyl methacrylate) macromonomer and acrylic acid



This multilevel record still has to incorporate the compromise shown for the macromonomer itself (see example

2.3), but the key difference between the structures of examples 2.5 and 3.4 is that the CNUM for the macromonomer (assume 234B, as before) will now appear in the online record, whereas previously this was not possible. Therefore, a search for the new structure

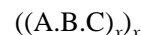
⇒ S 234B/CRN AND PMS/CI

will retrieve this comb polymer after the structure has been modified as shown. The enhancements will not affect the ability to retrieve only macromonomers, such as the one shown in example 3.4 (CNUM 234B), exclusive of comb polymers containing them. Thus, to find the CNUM for this macromonomer, the required search strategy will be

⇒ S ((123A AND 345C AND 456D)/CRN AND PMS/CI) NOT POLY-COMB-OR-GRAFT/CT

4. REGISTRATION OF MACROMONOMER HOMOPOLYMERS

As stated in section 3, the only situation for which multilevel registration fails is comb polymers prepared by homopolymerization of a macromonomer with no additional components such as a monomer or backbone end group. Thus, the format

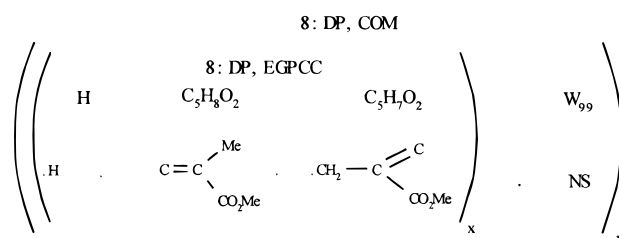


(wherein B is a monomer or an SRU and A and C are end groups) is rejected by the CASRS. To circumvent this problem, two possible solutions were considered; neither of them is ideal.

The solution adopted was to modify the unregistrable format ((A.B.C)_x)_x to the registrable format ((A.B.C)_x.D)_x. For this special situation, D is a *dummy* component that is added purely to enable registration; it has neither name nor molecular formula, and although it appears as a component of the structure, there is no indication of its presence in the polymer name. Macromonomer homopolymers containing the dummy component D carry the textual descriptor "DUMMY COMPONENT", which appears in the CT field in online displays. D is used *only* if no real backbone end groups are known; if at least one real end group is known and can be registered, D is not used.

Example 4.1 shows the new pictorial representation of the homopolymer (H(C₅H₈O₂)_xCH₂C(CO₂Me)=CH₂)_x obtained by polymerizing the macromonomer H(C₅H₈O₂)_xCH₂C(CO₂Me)=CH₂; Chart 3 shows how the online multilevel record for the homopolymer will appear.

Example 4.1. Structure keyed for multilevel, source-based representation in SCION of the homopolymer from poly-(methyl methacrylate) macromonomer (for the dummy component D, W₉₉ is the symbol keyed for "MF unspecified", and NS means "no stereochemical attributes")



The other solution considered was to modify the unregistrable format ((A.B.C)_x)_x to (A.(B)_x.C)_x (wherein B is a

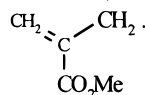
Chart 3. Online Multilevel Representation in SCION of the Homopolymer from Poly(Methyl Methacrylate) Macromonomer $H(C_5H_8O_2)_xCH_2C(CO_2Me)=CH_2$

CNUM: 121314M
 MF: ((C5 H8 O2 . C5 H7 O2 . H)x . Unspec)x
 DUP: POLY-(POLY-METHACRYLIC ACID, METHYL ESTER, END GROUP HYDRO, END GROUP 2-(METHOXYCARBONYL)ALLYL)
 CT: DUMMY COMPONENT; POLY-COMB-OR-GRAFT
 CI: PMS
 STE: 8:DP,COM

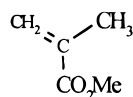
COM 1
 CNUM 111213L
 MF Unspec
 CI COM

COM 2
 CNUM 234B
 MF (C5 H8 O2 . C5 H7 O2 . H)x
 CI PMS, COM
 STE 8:DP,EGPCC
 COM 3
 CNUM 456D
 MF H
 CI COM
 STE 8:DP,FRA

.H
 COM 4
 CNUM 345C
 MF C5 H7 O2
 CI COM
 STE 8:DP,FRA



COM 5
 CNUM 123A
 MF C5 H8 O2
 CI COM



monomer and A and C are end group fragments). This fails to recognize the macromonomer as an entity; thus, registra-

tion would fail to create a CNUM for it, and the main advantage of the multilevel registration technique would be lost. This solution was therefore rejected.

5. CONCLUSIONS

CASRS single-level registration of comb polymer structures containing multicomponent macromonomers results in loss of identity of the macromonomer as a searchable entity. Until recently, the CASRS was believed by us to be incapable of registering a multilevel expression containing a source-based polymer within a source-based polymer. Newly acquired knowledge that the CASRS does, indeed, offer multilevel, source-based polymer registration suggested a way to enhance SCION chemical-file comb polymer records. Reregistration of a comb polymer as a multilevel, source-based expression creates, for each multicomponent macromonomer, a registration number that becomes an integral and *searchable* part of the overall comb polymer record.

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