Documentation and Indexing of C_4 Compounds: Pathways and Pitfalls[1]

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Although C_1 compounds exhibit "strange" and unique chemistry, their structural simplicity allows for straightforward description. Conversely, although the chemistry of C_4 compounds is more typical, description of the compounds, both by structure and by nomenclature, has not been so straightforward. Indexing errors for butanols are documented. Indexing and structure representation have been notably less than consistent for the butenes, and persistent errors are documented for butene monomers and polymers ("polybutenes") in products of several abstracting and indexing organizations.

INTRODUCTION

C_1 compounds are defined as those compounds containing carbon atoms that are not bonded to any other carbon atoms. Although not formerly singled out in descriptive organic chemistry, C_1 compounds have attracted much attention within the past decade, including several books[2a-c] and at least one journal.[2d] Of course, much of the interest has been in some specific C_1 compounds, especially methane, methanol, and formaldehyde. However, others, like formic acid, are distinctly more obscure than homologous related compounds. Although often considered the parent compounds of homologous series, C_1 compounds have been lately appreciated as distinct and even unique, not truly representative of the chemical family to which they are assigned. The common structural distinction, no additional bonds to carbon, is responsible for distinctly different, nonlinear, or even "strange" properties.

Methane, regarded as the "parent" of both the alkanes and the substituted aliphatics, has distinctive properties in comparison with other aliphatic hydrocarbons[3a,b] and melts at a temperature more than 50 °C higher than expected, in fact, even higher than propane. Its density is drastically less than that of any other hydrocarbon, and its bonds are distinctly less reactive than other hydrocarbon C–H bonds. The latter property is exemplified by an extremely high autoignition temperature.

Considering oxygenated derivatives, the C_2 compound ethanol is not generally appreciated to be toxic, but it is. However, that fact is overshadowed by the higher toxicity of methanol.[4a-c] This difference in toxicity is also the result of differing rates of metabolism of methanol and ethanol,[4c] as well as the additional differences in toxicity and metabolism of the higher oxidation products of each alcohol, namely, the respective aldehydes and carboxylic acids. Formaldehyde and formic acid are also both distinctly more toxic,[4a-c] and less easily metabolized, than are acetaldehyde and acetic acid, respectively.

In the study of homologous series of compounds, C_4 (butyl) compounds seem somehow more mundane. Properties become typical, i.e., more predictable, at or before C_4. Lower homologues are encountered more often and are inherently more interesting because they are unusual. For example, the following progression, not so apocryphal, is well-known to any chemist who has spent any appreciable time intentionally synthesizing, and derivatizing, biologically active compounds: "methyl, ethyl, butyl, futile..." (Anon.).

C_4 COMPOUNDS

The chemistry of C_4s may be more ordinary or typical, but the structure is decidedly more complicated. Progressing along homologous series, isomerism appears at C_2 for multiple substitution and at C_3 for single substitution (Figure 1). By the time one arrives at C_4, the situation becomes complicated.

Table I. Butanols[a]

name	structure	CAS Registry Number
1-butanol (*n*-butanol, butyl alcohol)	$CH_3CH_2CH_2OH$	71-36-3
isobutanol	$(CH_3)_2CHCH_2OH$	78-83-1
2-butanol (*sec*-butanol)	$CH_3CH_2CH(CH_3)OH$	78-92-2
tert-butanol (*t*-, tertiary butanol)	$CH_3C(CH_3)_2OH$	75-65-0
n-butanol (butyl alcohol)	$CH_3CH_2CH_2CH_2OH$	71-36-3
butanol	C_4H_9OH	35296-72-1

[a] The names isobutanol and *tert*-butanol do not conform to good nomenclature practice. They are included as primary entries for comparison only.

Table II. 2-Butanols

name	CAS Registry Number	name	CAS Registry Number
2-butanol	78-92-2	(*R*)-2-butanol	14898-79-4
(*S*)-2-butanol	4221-99-2	(±)-2-butanol	15892-23-6

Not only does the theoretical number of isomers begin to increase rapidly but, pragmatically, pure isomers are encountered more seldom. Mixtures of isomers become very common, especially for practical and commercial sources of materials. Chemical nomenclature, although fairly rigorous for pure isomers, becomes considerably less rigorous for substances commonly encountered.

For example, a list of the isomeric butyl alcohols is shown in Table I. Both *n*-butanol and isobutanol are primary alcohols. However, an error of perception is often made upon examination of the structure of secondary butanol (2-butanol). The branched chain is noted, and the compound is misattributed "isobutanol". Such errors can even creep into abstracting and indexing services. For example, in the past 20 years of *Chemical Abstracts*, more than 1700 documents have been indexed to *sec*-butanol and not to isobutanol. (Unless stated otherwise, use of Chemical Abstracts Registry Numbers (CASRN) was the search strategy of choice because of specificity of indexing. All searches were performed on the CAS ONLINE files as loaded on the STN network.) However, eight of those references are also indexed with the term "isobutanol". All but one are apparently misattributed to isobutanol because 2-butanol is indeed described. The remaining reference describes separation of isobutylene, isobutanol, and tertiary butanol, and the Registry Number for 2-butanol is apparently misassigned.

In addition, 2-butanol also occurs as two optically active stereoisomers and as the racemic mixture of the two, as shown

0095-2338/89/1629-0072$01.50/0

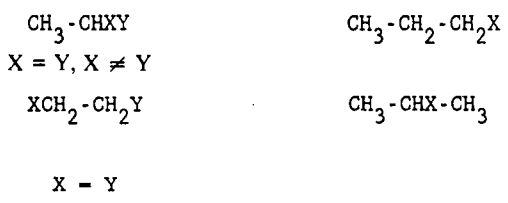

Figure 1. Onset of isomerism in substituted homologous alkane series.

Table III. Butenes

name	structure	CAS Registry Number
1-butene	$CH_3CH_2CH{=}CH_2$	106-98-9
2-butene	$CH_3CH{=}CHCH_3$	107-01-7
cis-2-butene	(*Z*)-$(CH_3)CH{=}CH(CH_3)$	590-10-1
trans-2-butene	(*E*)-$(CH_3)CH{=}CH(CH_3)$	624-64-5
isobutylene	$(CH_3)_2CH{=}CH_2$	115-11-7
butene	C_4H_8	25167-67-3

in Table II. Of course, 2-butanol can be assumed to be racemic, unless specified otherwise, so it might prove instructive to see how the CAS Registry Numbers for 2-butanol, unqualified and racemic, are assigned. Racemic 2-butanol (CASRN 15892-23-6) and 2-butanol (78-92-2) are not co-indexed, but 2-butanol is co-indexed 10 times each with (*R*)-(14898-79-4) and (*S*)- (4221-99-2) 2-butanol, for a total of 12 unique documents. Assuming that 2-butanol (78-92-2) is indexed when stereochemistry is not a factor, it would seem, in all cases, that the CASRN for 2-butanol is misassigned because all 12 references describe either resolution of 2-butanol, reactions with optically active reagents, or biochemical reactions.

For many series of isomers, CAS has a generic index name and Registry Number for which the exact description of isomerism is either not known, not described, or is indeed a mixture of the isomers. This system is also used for the butanols, as shown as the last item in Table I. As is the case for many aliphatic compounds, if butanol is described in an original reference, it probably means 1-butanol, the straight-chain primary isomer. However, in some cases, it might not, because the butanol in question might be encountered either as a known mixture, or a possible mixture, the isomeric content of which was not determined. An examination of 10 recent references indexed to butanol (35296-72-1) produced only 2 that seemed to describe mixtures of butanols. In addition, of the remaining eight references, two described physical properties, including gas chromatographic–mass spectral analysis, strongly suggesting that 1-butanol was described in the original document. Four references apparently describe the commercial product. In one of these, both 1-butanol (78-92-2) and butanol (35296-72-1) are indexed in a series of alcoholic reagents. The remaining two describe production of butanol by fermentation, the product of which is known to be 1-butanol.

Examination of 10 recent references indexed to 1-butanol (78-92-2) seemed to indicate correct assignment of the CAS Registry Number. However, the common name used in conjunction with the Registry Number, a policy begun in June 1987, was inconsistent. Names used, which are those used by the author, included butyl alcohol, 1-butanol, butanol, and *n*-butyl alcohol.

As the number of carbon atoms increases in the homologous series of olefins, stereoisomerism appears at C_4. A list of the butenes is shown in Table III. Note that specific stereoisomers, as well as the generic compound, are described for 2-butene.

STN CAS Registry file records for the butenes (1-butene, 2-butene, 2-butene double-bond stereoisomers) appear in Figures 2–5. Note that double-bond stereochemistry is indicated only in the nomenclature, but not in the structure (Figures 4 and 5). Additional listings include isobutylene (Figure 6) and butene (generic; Figure 7). In addition, note

```
RN  106-98-9
IN  1-Butene (8CI, 9CI)
SY  Butene-1
SY  .alpha.-Butylene
SY  1-Butylene
SY  Ethylethylene
SY  .alpha.-Butene
DR  33004-02-3, 1735-75-7, 54366-07-3
MF  C4 H8
CI  COM
LC  AGPAT, CASREACT, CSCHEM, DIPPR, PHARMPAT, TOXLIST, TSCA

EtCH :::::CH2

REFERENCES IN FILE CAOLD (PRIOR TO 1967)
4857 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 2.

```
RN  107-01-7
IN  2-Butene (8CI, 9CI)
SY  .beta.-Butylene
SY  Pseudobutylene
SY  .beta.-Butene
DR  1735-76-8
MF  C4 H8
CI  COM
LC  CASREACT, CSCHEM, TOXLIST, TSCA

MeCH :::::CHMe

REFERENCES IN FILE CAOLD (PRIOR TO 1967)
1229 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 3.

```
RN  590-18-1
IN  2-Butene, (Z)- (8CI, 9CI)
SY  cis-2-Butene
SY  cis-1,2-Dimethylethylene
SY  cis-Butene
SY  (Z)-2-Butene
SY  cis-Butylene
SY  .beta.-cis-Butylene
SY  cis-2-Butylene
SY  cis-butene-2
MF  C4 H8
CI  COM
LC  CASREACT, CSCHEM, DIPPR, PHARMPAT, TOXLIST, TSCA
ST  2:Z

MeCH :::: CHMe

REFERENCES IN FILE CAOLD (PRIOR TO 1967)
2790 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 4.

```
RN  624-64-6
IN  2-Butene, (E)- (8CI, 9CI)
SY  trans-2-Butene
SY  trans-1,2-Dimethylethylene
SY  trans-Butene
SY  (E)-2-Butene
SY  2-trans-Butene
SY  .beta.-trans-Butylene
SY  trans-butene-2
MF  C4 H8
CI  COM
LC  CASREACT, DIPPR, PHARMPAT, TOXLIST, TSCA
ST  2:E

MeCH :::: CHMe

REFERENCES IN FILE CAOLD (PRIOR TO 1967)
2474 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 5.

```
RN  115-11-7
IN  1-Propene, 2-methyl- (9CI)
SY  .gamma.-Butylene
SY  Isobutene
SY  Isobutylene
SY  2-Methylpropene
SY  iso-Butene
SY  Propene, 2-methyl- (8CI)
SY  Isopropylidenemethylene
SY  1,1-Dimethylethylene
SY  2-Methyl-1-propene
SY  2-Methylpropylene
MF  C4 H8
CI  COM
LC  AGPAT, CASREACT, CSCHEM, DIPPR, PHARMPAT, TOXLIST, TSCA

Me2C :::: CH2

REFERENCES IN FILE CAOLD (PRIOR TO 1967)
6234 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 6.

```
RN  25167-67-3
IN  Butene (8CI, 9CI)
SY  n-Butene
SY  Butylene
SY  n-Butylene
MF  C4 H8
CI  IDS, COM
LC  AGPAT, CASREACT, CSCHEM, TOXLIST, TSCA
ST  8:ID

    CM  1

    RN  106-97-8
    MF  C4 H10
    CI  COM

PrMe

2228 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 7.

that, because of nonindication of hydrogen, butene has the structure of butane, "PrMe" as shown, although shown as a component. Unlike other generic structures (specific isomerism not known or not shown), the lack of two hydrogens from the butane structure is not indicated. This can be very confusing, especially to a casual user or novice.

BUTENE POLYMERS

Note that the errors described above are relatively infrequent. However, upon examination of the butene polymers, confusion reigns, largely due to inadequate, inconsistent, or poorly described nomenclature used in the original publications. There is a variety of polymers with only butenes as components. They differ widely in properties, ranging from stereoregular crystalline poly(1-butene) to viscous, low molecular weight polymers primarily constituted of isobutylene monomers. The chief problem is that all tend to be called polybutenes, but there is no consistency in describing their composition. The following paragraph is paraphrased from the chapter on butylenes by Hoff et al.[5] in the *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed.

> There are three commercially important polymers derived only from butene monomers: stereoregular (crystalline, isotactic), poly(1-butene), polyisobutylene, and oligomeric polybutenes, which are usually termed polybutenes. This is the main source of confusion for two reasons: (1) the fact that they are low molecular weight oligomers is not always explicitly stated, and (2) their common name does not reflect that they are composed mainly of isobutylene monomeric units. In fact, they are prepared as oligomers from a mixed feed of all butene isomers, but the incorporation of 1- and 2-butene is quite low. They should be called polybutylenes because polybutene implies no incorporation of isobutylene. Uses are highly varied, but the common ones include blending components or chemical intermediates for automotive additives, especially motor oils, in addition to formulations of caulks, sealants, adhesives, coatings, and laminates.

Table IV. Butene Homopolymers

name	CAS Registry Number
isobutylene homopolymer	9003-27-4
1-butene homopolymer	9003-28-5
butene homopolymer	9003-29-6
1-butene homopolymer, isotactic	25036-29-7

Table V. 2-Butene Homopolymers

name	CAS Registry Number
2-butene polymers	25249-62-1
cis-2-butene polymers	25656-69-3
trans-2-butene polymers	25989-99-5

If early on a specific registry number had been assigned to a composition defined as "oligomeric polybutylenes, composed primarily of isobutylene units with the remainder other butene monomers", there would be far fewer problems. The second best choice would be "isobutylene, co-oligomer with 1- and 2-butene". At the very least, they could be indexed under polyisobutylene (CASRN 9003-27-4), since isobutylene is the predominant monomer. Viscous polybutenes could be indexed as "9003-27-4, low mol wt, ...", or "9003-27-4, liq, ...", and the higher molecular weight polybutenes could be indexed without qualification. However, over the years, oligomeric, or viscous, polybutenes have been indexed under most if not all of the butene "homopolymer" Registry Numbers, including the number for stereoregular poly(1-butene).

A list of the seven butene homopolymers is shown in Tables IV and V, including CAS Registry Numbers and trivial names, derived by searching the Registry File for the molecular formula $(C_4H_8)x$. The compositions in Table IV have the most references, and all have several references to many trade names listed as synonyms, including Indopol, Polyvis, and Hyvis (presumably trade names, but not attributed in the Registry File), all three of which appear as synonyms for both butene and isobutylene homopolymers. Searching these trade names produces even more listings, although most of the posted references are indexed with these four Registry Numbers.

Of the four compositions in Table IV, the one that most definitely should not be used for polybutenes is isotactic poly(1-butene) (CASRN 25036-29-7, Figure 8). Although an examination of 10 recent references indexed to this Registry Number produced no obvious misassignments, there have been errors in the past. Poly(1-butene) (9003-28-5, Figure 9) is also an incorrect number, and 2 of 10 recent references are probably misassigned. According to Hoff, polybutenes are actually polyisobutylenes, but the polyisobutylene number (9003-27-4, Figure 10) should probably be limited to higher molecular weight polyisobutylene. Of 10 recent references indexed to polyisobutylene (9003-27-4), 7 cover higher molecular weight polyisobutylene and 3 probably cover viscous polybutenes.

Because of the less definite description, butene homopolymer (9003-29-6) would be a better indexing point, but this listing has other problems. Structures are shown (Figure 11) for two components: butene and butane. This is an artifact of the manner in which butene itself is described, namely, with butane

```
RN  25036-29-7
IN  1-Butene, homopolymer, isotactic (9CI)
SY  1-Butene, polymers, isotactic (8CI)
SY  Poly-1-butene (isotactic)
SY  Isotactic poly(1-butene)
SY  Isotactic polybutene
SY  Isotactic 1-butene polymer
SY  Vestolen BT
SY  Vestolen BT 1711
SY  Isotactic poly(.alpha.-butene)
SY  Witron 0100
SY  Petrotex BUTUF-XB 100
SY  Witron 0400
SY  PB 4121
SY  Shell 0400
SY  PB 0400
SY  PB 4125
MF  (C4 H8)x
CI  PMS
LC  CSCHEM
ST  8:PM,ISOTACTIC

    CM  1

    RN  106-98-9
    MF  C4 H8
    CI  COM

EtCH :::::CH2

264 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 8.

Table VI. Butene "Oligomers"

name	CAS Registry Number	name	CAS Registry Number
1-butene dimer	6993-22-2	isobutylene trimer	7756-94-7
1-butene trimer	82983-62-8	isobutylene tetramer	15220-85-6
1-butene tetramer	82983-64-0	isobutylene pentamer	42278-27-3
1-butene pentamer	82983-65-1	isobutylene hexamer	85578-98-9
1-butene hexamer	82983-60-6	butene dimer	9021-92-5
1-butene heptamer	82983-61-7	butene trimer	72317-18-1
1-butene octamer	82983-63-9	butene tetramer	83602-47-5
1-butene nonamer	82983-66-2	2-butene dimer	24993-12-2
isobutylene dimer	18923-87-0	(*Z*)-2-butene dimer	85097-21-8

Table VII. Butene "Oligomers"—SRU

name	CAS Registry Number
poly(butylidene)	26967-02-2
poly(1,1-dimethyl-1,2-ethanediyl)	25038-49-7
poly(1-ethylethylene)	25038-50-0
poly(1,2-dimethylethylene)	32167-46-7

as a component. Again, this can be confusing, especially when this substance is used to index the product of a stream of mixed butenes and butane. A novice could infer that butane is incorporated into the polymer.

In addition, there are 18 listings for butene dimers through nonamers (Table VI) and 4 listings for compositions of $(C_4H_8)n$ (Table VII), which are all SRU, or structural repeating unit, polymers or oligomers of the butenes. (Sample compound records are shown in Figures 12 and 13.) Some of these are possible listings for the oligomeric polybutenes. Examination of most of the references shows appropriate indexing for the most part. A notable exception occurs when the trimer, tetramer, and pentamer of 1-butene are indexed as products of the oligomerization of a mixture of isobutylene and 1-butene, with obvious predominant incorporation of isobutylene.

Hoff describes the polymerization reactivity of butenes as isobutylene ≫ 1-butene > *cis*-2-butene > *trans*-2-butene (unreactive) with Lewis acid or cationic catalysts or initiators.[5]

```
RN  9003-28-5
IN  1-Butene, homopolymer (9CI)
SY  1-Butene, polymer (8CI)
SY  Poly(1-butene)
SY  Poly-.alpha.-butylene
SY  Mobil PB 103
SY  .alpha.-Butylene polymer
SY  PB 103 (polymer)
SY  PB 103
SY  PB 001
SY  PB 003
SY  PB 004
SY  Witron
SY  PB 630
SY  PB 1200
SY  Witron 1200B
SY  Nitron 100
SY  Poly-.alpha.-butene
SY  PB 8640
SY  Witron 6400
SY  M 801
SY  WBS 139
SY  BR 200
SY  PB 1600SA
SY  PB 1710SA
SY  PB 8340
SY  PB 200
SY  M 8010
SY  M 0400
SY  KHT 712
SY  Duraflex 0110
SY  Duraflex DP 1520
SY  Duraflex DP 1560
MF  (C4 H8)x
CI  PMS, COM
LC  AGPAT, CSCHEM, PHARMPAT, TOXLIST, TSCA

    CM  1

    RN  106-98-9
    MF  C4 H8
    CI  COM

EtCH :::::CH2

1232 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 9.

Table VIII. Butene Polymers: Two-Component

name	CAS Registry Number
1-butene/2-butene polymer	28602-88-2
1-butene/*cis*-2-butene polymer	28517-07-9
isobutylene/*cis*-2-butene polymer	27119-30-8
1-butene/isobutylene polymer	26938-45-4
isobutylene/*trans*-2-butene polymer	26938-44-3
isobutylene/2-butene polymer	25687-04-1
butene/isobutylene polymer	9044-17-1

Table IX. Butene Polymers: Three-Component

name	CAS Registry Number
1-butene/*cis*-2-butene/isobutylene	92900-30-6
1-butene/*cis*-2-butene/*trans*-2-butene	51290-18-7
1-butene/2-butene/isobutylene	28300-07-4
1-butene/*cis*-2-butene/*trans*-2-butene/isobutylene	9043-61-2

Even though the incorporation of 1-butene and 2-butene is low in polybutenes, they can be realistically defined as butene copolymers. To some extent, polybutenes have been indexed as copolymers containing two, three, or four butene components. Of the seven two-component polymers (Table VIII), five incorporate 2-butene and all are used for polybutenes, inappropriately for the latter. However, the remaining two

```
RN  9003-27-4
IN  1-Propene, 2-methyl-, homopolymer (9CI)
SY  Isobutylene resin
SY  Polyisobutylene
SY  Propene, 2-methyl-, polymers (8CI)
SY  Oppanol B
SY  Paratac
SY  Polyisobutene
SY  P 118
SY  Poly(2-methylpropene)
SY  Indopol H 1900
SY  Isobutene polymer
SY  Isobutylene polymer
SY  Oppanol B 15
SY  PIB 100
SY  Polyisobutylene PSG
SY  2-Methylpropene polymer
SY  Hyvis 200
SY  Oppanol B 3
SY  P 85
SY  Isobutylene homopolymer
SY  Polyvis 200SH
SY  Polyvis 150SH
SY  Polyvis 30SH
SY  Amoco 600
SY  Maxvis 2000
      .
      .
SY  Isobutene homopolymer
SY  Hyvis 30
      .
      .
SY  Lubrizol 5183
SY  Lubrizol 3174
SY  Oppanol B 230
SY  Chevron 32
SY  Chevron 24
SY  Polyvis 025SH
SY  Napvis 10
SY  P 118N
ADDITIONAL NAMES - UNAVAILABLE FOR DISPLAY
DR  53571-24-7, 78361-91-8, 64104-22-9, 51810-32-3, 39323-31-4
MF  (C4 H8)x
CI  PMS, COM
LC  AGPAT, CSCHEM, PHARMPAT, TOXLIST, TSCA

    CM  1

    RN  115-11-7
    MF  C4 H8
    CI  COM

Me2C :::: CH2

4462 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 10.

copolymers, butene/isobutylene (9044-17-1) and isobutylene/1-butene (26938-45-4), are definitely appropriate.

Of the three-component polybutenes (Table IX), one indicates a realistic composition for a viscous polybutene: copolymer of isobutylene, 1-butene, and *cis*-2-butene (92900-30-6). It is used exactly once, interestingly enough, for an Amoco process patent. One other is adequate: polymer of isobutylene, 1-butene, and 2-butene (28300-07-4) is used for both high and low molecular weight polymers in 20 references. The third is a polymer of 1-butene with *cis*- and *trans*-2-butenes and is used inappropriately for viscous polybutenes in six of seven references. In many of the references indexed to the multi-butene copolymers, single-component polybutenes are also indexed, possibly as a hedge.

Searching "polybutene" both as text and abstract terms yields over 2100 references. Upon examination, recent references exhibit a variety of names assigned in Registry Number indexing, including butene polymer, 1-butene polymer, and more.

Amoco Chemical has been primarily interested in low molecular weight polybutenes, and it would be interesting to check how Amoco-authored references are indexed. Of 64 references, most are indexed to butene homopolymer (9003-29-6; acceptably vague) with a few instances of polyisobutylene (9003-27-4) and butene–isobutylene copolymer (9044-17-1; both acceptable), poly(1-butene) (9003-28-5; unacceptable),

```
RN  9003-29-6
IN  Butene, homopolymer (9CI)
SY  Butene, polymers (8CI)
SY  Amoco 15H
SY  Indopol H 100
SY  Indopol
SY  Polybutene SH 015
SY  Polybutylene
SY  Butene polymer
SY  Oronite 6
SY  Indopol H 300
SY  Chevron 16
SY  Petrofin 100
SY  Indopol 1900
      .
      .
SY  Hyvis 7000/45
SY  Hyvis 07
SY  Indopol L 14
SY  Indopol L 100
SY  H 100
SY  H 300
SY  L 14
SY  L 100
SY  Amoco H 300
SY  H 1500
SY  LV 50
SY  H 1900
SY  Polyvis 2000CH
SY  L 14 (polymer)
SY  Witron 131
      .
      .
ADDITIONAL NAMES - UNAVAILABLE FOR DISPLAY
DR  11121-22-5, 9037-04-1, 42612-15-7, 52012-58-5
MF  (C4 H8)x
CI  PMS
LC  AGPAT, CSCHEM, PHARMPAT, TOXLIST, TSCA

    CM  1

    RN  25167-67-3
    MF  C4 H8
    CI  IDS, COM
    ST  8:ID

        CM  2

        RN  106-97-8
        MF  C4 H10
        CI  COM

PrMe

1415 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 11.

```
RN  82983-66-2
IN  1-Butene, nonamer (9CI)
MF  (C4 H8)9
CI  PMS

    CM  1

    RN  106-98-9
    MF  C4 H8
    CI  COM

EtCH :::::CH2

1 REFERENCES IN FILE CA (1967 TO DATE)
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Figure 12.

and a few other misinterpretations. Several references have no relevant Registry Number indexed, but some have the

```
RN  32167-46-7
IN  Poly(1,2-dimethylethylene) (8CI)
MF  (C4 H8)n
CI  PMS
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
1 REFERENCES IN FILE CA (1967 TO DATE)
```

Figure 13.

Registry Number for butene polymer listed in the abstract. Curiously, one reference has the number for poly(1-butene) (9003-28-5) in the abstract and that for butene polymer (9003-29-6) in the index.

One Amoco polybutene reference was indexed with a phrase linking butene, as the Registry Number, with "polymer" (25167-67-3, polymer). This combination, or the related one using the derivative form (25167-67-3D, polymer), is used 11 times. Seven of the references definitely involve viscous polybutenes.

As a result of the confusion on assignment of Registry Numbers, it is very difficult to search comprehensively for polybutenes with any acceptable degree of relevance. One method of improving relevance is to simultaneously search for common uses of oligomeric polybutenes, but this always causes doubt as to the comprehensiveness of the search. Ironically, uses or other context usually provides good clues for which of several compositions is being described. For example, the various polybutene Registry Numbers were searched for references referring to lubricants or lubrication. Of 10 recent references, all dealt with polybutenes, and all were indexed to polyisobutylene, butene homopolymer, and butene–isobutylene copolymer.

The confusion on polybutenes is not limited to *Chemical Abstracts*. PROMT, the marketing abstracts file produced by Predicasts, has two Standard Industrial Code (SIC) product codes that are relevant to the issue. SIC code 282144 is titled "polybutene plastics" and should be reserved for high molecular weight poly(1-butene) or polyisobutylene. Recent abstracts show that this is the case, but of over 90 postings, at least 13 actually describe viscous polybutene, including uses as adhesives and tackifiers. An SIC code, 2864991, also exists for polybutenes, which should be used for all other polybutenes. However, at least 6 of 74 references describe crystalline poly(1-butene), which would be properly indexed as "polybutene plastics" (SIC 282144), with uses such as in pipe and film. For several abstracts in both categories, not enough additional information is given to determine whether or not the correct code is assigned.

An interesting trend was discovered when uses of polybutenes were examined in context for determining accuracy of polybutene indexing in PROMT. Crystalline poly(1-butene) is now being used in hot-melt adhesive formulations, so that the combination of polybutene and adhesive no longer necessarily indicates viscous polybutenes.

The Central Abstracting and Indexing Service of the American Petroleum Institute (API) has an excellent controlled indexing system, based on a continually updated thesaurus, featuring product and reactant roles plus autoposted chemical component terms for indexed chemicals, including some polymers. Since polymers of isobutylene (2-methylpropene) and 1-butene are the only butenes indexed as such within the system, probably the most appropriate indexing phrase would be the linked combination of 2-methylpropene copolymer and 1-butene copolymer. Use of oligomer or some other indication of relatively low molecular weight would be desirable, but API limits the use of oligomer to polymers of less than seven monomer units. However, inspection of the nine postings in the API Literature file for articles indexed to polybutene(s) and involving Amoco reveals exclusive use of homopolymer index phrases for the polybutene concept. Individual homopolymer

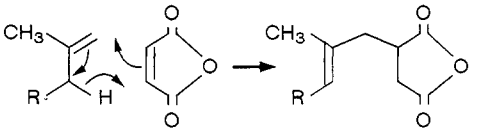

Figure 14. Ene reaction.

phrases for isobutylene plus 1- and 2-butenes are indexed twice, with links, and the combination of 1- and 2-butene is indexed six times. The latter is unrealistic at best, and the whole concept of indexing copolymers as linked homopolymers seems strange. Use of the free-text term "polybutene", and its plural, seems to be the most effective way to search polybutenes in the API files.

Two series of chemical index fragment coding are used to index the Derwent World Patent Index files (WPI). Proprietary codes exist for polymers of 1-butene and isobutylene within the PLASDOC (polymers and plastics) portion of WPI, which covers patents on polymers and plastics from more than 24 countries. The codes can be linked to additional codes for the concepts of homopolymer and oligomer as appropriate. Twelve Amoco polybutene patents were examined for indexing of the polybutene concept. Polymers of 1-butene were indexed in four cases, and both poly(1-butene) and butene polymer were indexed eight times.

Additionally, problems occur with indexing of reaction products of the polybutenes. Typically, advantage is taken of the terminal double bond of viscous polybutenes and the ene reaction used to alkylate dienophiles such as maleic anhydride (Figure 14). Although structures of the resulting alkyl succinates (or alkenyl succinates) are reasonably well-known, they typically do not appear in the Registry File. However, the situation is so complex it warrants an additional paper and will not be discussed further at this time.

Although difficulties probably exist with description of other butene polymers, I have only examined one additional case: linear low-density polyethylene (LLDPE). Classical low-density polyethylene was discovered to have hydrocarbon branches in the polymer chain, with ethyl, or 2-carbon-atom, branching the most predominant. Within the past decade, LLDPE was developed, which involves the polymerization of ethylene with α-olefins, primarily 1-butene. The incorporation of butene is about 5%, but LLDPE has been indexed to ethylene homopolymer (9002-88-4) in the majority of cases (130 of 241). The total was determined by a term search for LLDPE or linear low-density polyethylene. An additional 69 references are indexed to ethylene/1-butene copolymer (25087-34-7, Figure 15) and 9 to ethylene/butene copolymer (9019-29-8, Figure 16). Of the 29 references indexed to both polyethylene and ethylene/1-butene copolymer, only 4 are improperly coded with both Registry Numbers because only LLDPE is described. The remainder describe both "regular" polyethylene and linear low-density polyethylene, either as separate entities, blends, or mixtures.

It should be obvious that LLDPE requires a unique Registry Number and should not be indexed as polyethylene. Linear low-density polyethylene is an adequately described copolymer. Granted, higher α-olefins can be used, but marketing information indicates that 1-butene is used predominantly in the production of LLDPE. Unique Registry Numbers exist for the other copolymers that have been described and should be used when appropriate. Multiple Registry Numbers should only be used in such cases when both species are described in the document, not as a hedge to modify the usage of the primary polymer, in this case, polyethylene. At any rate, improper use of the Registry Number for polyethylene is particularly onerous because the searcher must literally look for the needle in the haystack, because polyethylene (as 9002-88-4) has over 55 000 references.

```
RN  25087-34-7
IN  1-Butene, polymer with ethene (9CI)
SY  Ethylene, polymer with 1-butene (8CI)
SY  1-Butene, polymer with ethylene (8CI)
SY  Ethylene-1-butene copolymer
SY  1-Butene-ethylene copolymer
SY  Ethene, polymer with 1-butene (9CI)
SY  Marlex 5003
SY  Petrothene LB 733
SY  Ethylene-1-butylene copolymer
SY  Ethylene-1-butene polymer
SY  1-Butene-ethylene polymer
SY  Marlex 5002
SY  1-Butene-ethene copolymer
SY  1-Butene-ethene polymer
SY  Carlona 40-045/09
SY  .alpha.-Butylene-ethylene polymer
SY  Sclair 96A
SY  Sclair 14B
SY  Sclair 11K
SY  .alpha.-Butene-ethylene copolymer
SY  .alpha.-Butylene-ethylene copolymer
SY  Witron 8240-2
SY  Bakelite GRSN 7040
SY  Sclair 35B
SY  HO 60-45P
SY  Sclair 51-35B
SY  Sclair 11P
SY  Neozex 3510F
SY  Bakelite GRSN 7144


ADDITIONAL NAMES - UNAVAILABLE FOR DISPLAY
DR  102381-57-7, 88984-97-8, 81859-72-5, 27082-52-6
MF  (C4 H8 . C2 H4)x
CI  PMS
LC  AGPAT, CHEMLIST, PHARMPAT, TSCA

    CM  1

    RN  106-98-9
    MF  C4 H8
    CI  COM

EtCH :::::CH2


    CM  2

    RN  74-85-1
    MF  C2 H4
    CI  COM

H2C ::::CH2

2134 REFERENCES IN FILE CA (1967 TO DATE)
```

Figure 15.

In summary, I have attempted to show that increasing complexity of chemical structure rapidly increases both the complexity of description or nomenclature and the number of possibilities for error. As demonstrated earlier, errors in indexing are infrequent for the monomers but become all too common for the polymers. The differences in properties between C_1 and higher homologues were emphasized to reinforce the following rules for classification and indexing: just as substances with different structures are considered distinct, substances of similar structure, but with differing properties, should be considered distinct entities and indexed accordingly.

```
RN  9019-29-8
IN  Butene, polymer with ethene (9CI)
SY  Ethylene-butene copolymer
SY  Ethene, polymer with butene (9CI)
SY  Butene-ethylene copolymer
SY  Butene-ethylene polymer
SY  Butylene-ethylene polymer
SY  Ethylene-butene polymer
SY  Butene, polymer with ethylene (8CI)
SY  Ethylene-butylene copolymer
SY  Butylene-ethylene copolymer
DR  9040-66-8
MF  (C4 H8 . C2 H4)x
CI  PMS
LC  AGPAT, CHEMLIST, PHARMPAT, TSCA

    CM  1

    RN  74-85-1
    MF  C2 H4
    CI  COM

H2C ::::CH2


    CM  2

    RN  25167-67-3
    MF  C4 H8
    CI  IDS, COM
    ST  8:ID

        CM  3

        RN  106-97-8
        MF  C4 H10
        CI  COM

PrMe

275 REFERENCES IN FILE CA (1967 TO DATE)
```

Figure 16.

By covering several sources, the attempt has been made to show how pervasive the problems are. Of course, these inaccuracies not only breed user frustration but tend to further propagate the errors. All criticisms are meant to be constructive and should be taken with that in mind.

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