The following search conditions will be used:

BFE = CO——CO *

AFT = CC-BOND * 2 TIMES ALCOHOL(A) * (R)-

(The conditions which are described for AFT with standardized terms mean that the ring closure (R-; any ring size possible) is accomplished by formation of a CC-BOND with two alcohol groups (2 TIMES ALCOHOL(A)) on the ring.)

The search gives the printout in Figure 10 and the Synthesis Abstract in Figure 11.

ACKNOWLEDGMENT

Thanks are due to the many colleagues, most of them young chemists, especially to Dr. H. Scherrer, for their collaboration and to Mr. Margadant for writing the successful computer programs.

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# Chemical Reactions Information Retrieval from Chemical Abstracts Service Publications and Services†

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Received March 20, 1979

Information on chemical reactions in general and on specific reactions such as oxidation may be found by searching CAS publications and services. Using common or author terminology, the searcher relies on the Keyword Index in the weekly issues of *Chemical Abstracts* (CA) for current awareness. Having consulted the cross-references and indexing notes in the Index Guide, the searcher accesses the controlled set of terms in the General Subject Index for in-depth and retrospective searching. In this index, the searcher finds reaction headings and headings related to reactions such as technological processes and classes of compounds. The Index Guide also includes a hierarchy of reaction headings to help the searcher choose the most appropriate heading. Reactants, intermediates, and products found in the Chemical Substance Index provide access to reactions as well. The entries in these indexes lead the searcher to the abstracts for further information concerning the primary documents in which the study was reported. Two examples of searching for reactions are given.

In the introduction to the First Decennial Index of *Chemical Abstracts* (CA), E. J. Crane, the Editor, wrote ". . . it is obvious that this First Collective Subject Index to the journal should be not only accurate and thorough but that it should also be so prepared and arranged that those who use it can find all of the references on the various subjects with certainty and with a minimum of effort". This statement, made in 1919, is still valid today, and the policies implicit in it lead to complete, accurate, consistent, and rational indexing of all that is new and significant in chemistry and chemical engineering. What holds true for chemistry in general holds also for reactions in particular.

The First Decennial Index had many entries for different types of reactions. There were, for example, about 280 entries at **Oxidation**, 190 at **Rearrangements**, and 70 at **Substitution**. The concept of cross-referencing was used: the Beckmann rearrangement was cross-referenced to **Rearrangements**, and at **Condensation** one was additionally directed to such specific headings as **Claisen condensation** and **Friedel-Crafts reaction**.

In addition to reactions, classes of compounds, such as amines, have also been indexed since the beginning of CA. These headings, together with the text that accompanies and expands upon them, provide additional access to reaction information. An entry in the First Decennial Index, for example, reads "**Amines**, addition reaction with diazonium salts". The entries for specific chemical substances also provide useful information about reactions that sometimes cannot be found at other entries. For example, starting compounds and intermediates, which are particularly valuable entries, have been extensively indexed since 1973.

It is obvious from this brief introduction that CAS publications and services can readily answer questions that can be expressed in terms of rather general reactions or classes of compounds. Questions that can be expressed in terms of specific compounds, whether such compounds are reactants, intermediates, or products, can also be answered easily.

Questions expressed in terms of structural moieties or substructures, or in terms of bonds broken and made, on the other hand, can be answered only with difficulty. If the searcher wants to know about reactions that involve a transformation of one substructure to another, the searcher must express that question either at a more specific level by thinking of a specific substance, or at a more general level by fitting it to a reaction heading or a compound class heading. The latter can be used if a substructure fits one or more such headings, but not all substructures correspond to index headings.

## SEARCH FOR INFORMATION USING A GENERAL SEARCH QUESTION

Two questions, a general one and a specific one, will be explored to demonstrate how a searcher can use CAS publications and services to retrieve information about chemical reactions. The search strategy illustrated leads the searcher to the Keyword Index, and to the General Subject Index and

† Presented in the symposium, "Retrieval, Analysis, and Indexing of Chemical Reactions", 176th National Meeting of the American Chemical Society, Miami Beach, Fla., Sept 12, 1978.

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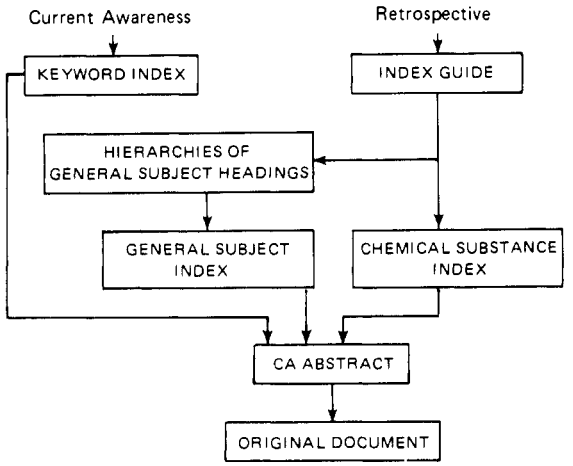



**Figure 1.** Search strategy.

Alkene
carbene cycloaddn kinetics 146047e
codimerization carbonylation 146329y
cyclization MO 146214g
disproportionation review 146324t
elimination alkylborabicyclononane aldehyde 146956a
➤ epoxidn trioxolene 146173t
homogeneous hydrogenation catalyst 146134f
hydroxylation osmium catalyst P 146413w
➤ oxidn catalyst adsorption 146336y
➤ oxidn catalyst molybdate 146338a
stannyl prepn isomerization 146461k 146964b
Alkoxide
•
•
•
Epoxidn
➤ alkene trioxolene 146173t
➤ chloropropene metal salt 146342x
cyclohexene hydroperoxide molybdenum 146161n
indenone 146807c
menthene 147060r
➤ olefin arsenic catalyst P 146750d
➤ propylene 146678m
➤ styrene P 146748j
Epoxy
•
•
•
Olefin
acetylacetonatonickel reaction 147041k
➤ epoxidn arsenic catalyst P 146750d
hydration phosphoric acid catalyst P 146410t
hydroformylation P 146420w P 146427d
hydroformylation rhodium catalyst 146328x
lower oligomerization P 146403t
➤ oxidn tin antimony catalyst 146336y
purifn partial hydrogenation P 146404u
toluene alkylation P 146585d
•
•
•

Oxidn
acenaphthene deriv dichromate 146179z
acetaldehyde metal salt 146342x
acetaldehyde peroxide promotion P 146430z
➤ acrolein cobalt molybdate catalyst 146375k
➤ alkene catalyst molybdate 146338a
alkoxyphenylpropionate 146717y
allylic cholestenone 147136v
amino acid Pseudomonas 143183k
amino alc ozone 146560a
ammoxidn catalyst furan review 146670c
anodic aluminum education 145837a
➤ anodic propylene pH 146351z
arylmethylenethioflavone 146292f
benzyldihydronicotinamide cupric ion 146721v
butanone ozone mechanism 146376m
butyraldehyde kinetics mechanism 146138k
carboxylate cerium 146170q
catalyst methanol P 146421x
•
•
•
esterification acrolein methanol 146383m
➤ ethylene catalyst kinetics 146367j
eudesmenolide 147077b
glucose P 147191j
hydrazobenzene kinetic differentiation 146136h
hydrocarbon catalytic review 145909a
iron ferritin mechanism 142107b
irradn linseed oil 145326h
isobutylphenylpropanol P 146617r
ketone kinetics 146152k
•
•
•
nitrotoluene ozone mechanism 146175v
➤ olefin tin antimony catalyst 146336y
org uranium hexafluoride 146559y
Paracoccus phosphorylation electron transport 143034n
paraffin product viscosity 145955n
penicillin cephalosporin 146853q
phase transfer alc 146359h
phenol iron phenanthroline 146157r
photochem phenanthrylphenylbutenyne 146140e
polyalkylbenzene resin nitric acid 146565x
➤ propylene acetic acid 146385p
➤ propylene ammonia catalytic 146339b
➤ propylene catalyst 146337z
● propylene molybdenum IR 146160m
pyruvate ferredoxin flavodoxin 142007u
ruthenium arylalkylamine 147201n
stability sunflower oil 145306b
stabilization edible oil P 145402e
stigmastadienol 147134t
terpene 147064v
➤ terpene allylic alc 147059x
toluene nitrogen compd 146583b
xylene catalyst shape P 146625s

**Figure 2.** Keyword Index.

the Chemical Substance Index by way of the Index Guide (Figure 1). The discussion will be confined primarily to printed publications with only passing references to computer-readable services.

**Formulation of a General Search Question.** A searcher can formulate a general question to search for both current awareness and retrospective information about reactions. One example of such a search can be illustrated by considering the question, "What new information has been published recently about the oxidation of olefins and related compounds?" We use this question in the first part of this paper to illustrate the procedure a searcher would follow to find answers to a general search question about reactions.

Olefins, or alkenes, are a very large group of compounds that includes such important chemicals as ethylene, propylene, acrolein, vinyl chloride, cyclohexene, and styrene. Their oxidation can produce oxides, glycols, aldehydes, ketones, acids, or cyclic compounds, and may be accomplished by a variety of reagents. Depending on the reagents and products, the oxidation may, in fact, be better described as ozonization, peroxidation, or epoxidation. To obtain the desired information on topics such as these, therefore, it is obvious that the searcher must state the initial question carefully, using words as specifically or as generally as necessary. The searcher also must be flexible enough to alter the nature or the scope of the question as the search proceeds if it is not producing the desired information.

**The Keyword Index.** Once the question has been properly formulated, the searcher begins the search with the weekly issues of CA. The searcher chooses the terms that relate to the subject of the question to examine the Keyword Index contained in each issue of CA.

To find information related to our search question, we might choose terms such as the reaction term "oxidation" and the compound class terms "olefin" and "alkene". We would then turn to the Keyword Index, which contains keyword phrases arranged in alphabetic order. If we choose a recent issue of CA and look at entries under "Oxidn", "Alkene", and "Olefin", we find among many entries such relevant ones as those highlighted in Figure 2. [The indentation for easy scanning and the capital P for patent preceding the abstract number were introduced into the Keyword Index in July 1978 with Volume 89. The Keyword Index employs the singular form and the full set of CAS abbreviations.] The redundancy in entries, for example, "Oxidn alkene catalyst molybdate" and "Alkene oxidn catalyst molybdate", is deliberate, allowing searchers to find information at a variety of access points.

At the "Oxidn" heading we can look for specific examples of alkenes such as propene or isoprene, or we can extend the reaction terms to cover other oxidations, such as epoxidation (Figure 2). Searchers can continue to add terms, depending on what other words they find at the keyword entries or in the abstracts they consult, until they are satisfied that they have exhausted all possibilities.

A searcher should keep in mind, however, that the Keyword Index is not collected in a Volume Index and, hence, is most often used as a weekly current-awareness tool, although it also has some value in retrospective searching. The words used as entries in the Keyword Indexes are derived from the title, text, and context of the abstract. They tend to be words used by the author, often translated or transliterated from a foreign language. Because no major effort has been made to standardize these terms or to use consistent synonyms or systematic nomenclature for concepts or substances, the terms do not provide as complete a guide to the source document as do the entries in the Volume Indexes.

**The CA Condensates Search Aid Package.** It is not always obvious what terms to use in searching the Keyword Index. The searcher can consult the *CA Condensates* Search Aid Package, however, for aid in devising useful search terms. This search aid package, available on microfiche or microfilm, was created to help those who use *CA Condensates*, the computer-readable counterpart of the Keyword Index. The package includes the Word Frequency List and the Key-Letter-In-Context (KLIC) Index.

The Word Frequency List is an inventory of about 220 000 unique words appearing in document titles and keywords in *CA Condensates*. The list indicates the number of times each word occurs. Words that occur more than ten times in the Word Frequency List are segmented at each letter except the

| | | |
|---|---|---|
| ISOPER | OXIDASES | 15 |
| | OXIDATE | 14 |
| PER | OXIDATIC | 11 |
| | OXIDATION | 6072 |
| DE | OXIDATION | 162 |
| RE | OXIDATION | 16 |
| SULF | OXIDATION | 14 |
| ANTI | OXIDATION | 11 |
| AMM | OXIDATION | 77 |
| CO | OXIDATION | 37 |
| ELECTRO | OXIDATION | 44 |
| PHOTO | OXIDATION | 166 |
| AUTO | OXIDATION | 12 |
| EP | OXIDATION | 170 |
| PER | OXIDATION | 106 |
| AUT | OXIDATION | 219 |
| | OXIDATIONS | 108 |
| | OXIDATIVE | 2037 |

**Figure 3.** KLIC Index.

**Oxidation**
Studies of oxidation, the reaction that involves valence increase, electron loss, oxygen addition to molecules, etc., are indexed at this heading when original document especially emphasizes the process or some aspect of it, e.g., mechanism. Other studies of oxidation are indexed at headings for the substances involved. Treatment with oxygen when reaction is not emphasized is indexed at *Oxygenation*
See also
*Electron exchange*
*Reduction*
agents——see *Oxidizing agents*
amm——see *Ammoxidation*
aromatization——see *Aromatization*
catalysts——see *Oxidation catalysts*
chlorination and——see *Oxychlorination*
in corrosion——see *Corrosion* and headings for specific alloys and metals
in corrosion prevention——see *Corrosion prevention* and headings for specific alloys and metals
dehydrogenation——see *Dehydrogenation*
diazotization——see *Diazotization*
in disproportionation——see *Disproportionation*
elec. potential of——see *Electric potential, oxidn.*
electrochem.——see *Oxidation, electrochemical*
enthalpy of——see *Heat of oxidation*
➤ epoxidn.——see *Epoxidation*
haloform——see *Halogenation, haloform*
kinetics of——see also *Kinetics of oxidation*
in metab.
see
*Animal metabolism*
*Plant metabolism*
by nitrification——see *Nitrification*
➤ ozonization——see *Ozonization*
➤ per——see *Peroxidation*
by phosphorylation——see *Phosphorylation, biological*
photochem.——see *Oxidation, photochemical*
prevention of, agents for——see *Antioxidants*
prevention of, coatings for——see *Coating materials*
redn.——see *Redox reaction*
Serini——see *Rearrangement, Serini*
of sewage and wastes——see *Waste* headings
susceptibility to——see *Oxidizability*
in tarnishing——see *Tarnishing*
**Oxidation, electrochemical**
anodization by——see *Anodization*
catalysts——see *Oxidation catalysts, electrochem.*
elec. potential of——see *Electric potential, oxidn.*
electrolysis——see *Electrolysis*
enthalpy of——see *Heat of oxidation*
kinetics of——see also *Kinetics of oxidation*
**Oxidation, photochemical**
catalysts——see *Oxidation catalysts, photochem.*
enthalpy of——see *Heat of oxidation*
kinetics of——see also *Kinetics of oxidation*

**Figure 4.** Index Guide.

last, and the fragments thus derived are alphabetized to form the KLIC Index, a useful tool for devising search terms (Figure 3). The KLIC Index helps searchers find additional search terms by allowing them to look for embedded terms. For example, the KLIC Index entries positioned around the term "oxidation" include such terms as "ammoxidation", "photooxidation", and "autoxidation", all, some, or none of which may be included in the keyword search.

**The Index Guide.** Before discussing the Volume Indexes, which are the traditional sources of retrospective searching, it is important to mention the Index Guide, without which a searcher cannot use the Volume Indexes efficiently. The Index Guide is an invaluable aid in finding terms that should be included in any search strategy. It directs the searcher to appropriate search headings in the Chemical Substance and General Subject Indexes.

The main body of the Index Guide is a collection, arranged

**Alkenes**
Studies of olefins as a class are indexed at this heading. For specific alkenes, see such headings as *1-Propene, 2-Propenoic acid*. In the absence of functions expressed as suffixes, specific unsaturated hydrocarbons with cyclic components are indexed at the preferred ring, e.g., *Benzene, 1,1'-(1,2-ethenediyl)bis-* (formerly *Stilbene*); *Benzene, ethenyl* (formerly *Styrene*). Acyclic olefinic hydrocarbons with branched chains are indexed at the headings which express in descending order of preference: (a) longest chain, (b) maximum number of multiple bonds, (c) maximum number of double bonds, (d) lowest-numbered locants in parent compound, (e) maximum number of substituents, (f) lowest-numbered locants for substituents on parent compound, or (g) earliest index position of complete name. E.g., *Nonane, 5-(1-propenyl)-; 1,3-Butadiene, 2-methyl-* (formerly *Isoprene*); *1-Propene, 3-chloro-2-(chloromethyl)-2-methyl-; 1,3,7-Nonatriene, 5-(2-butynyl)-*
See also *Ethene, derivatives (general)*
acetylenic
see such headings as
*Alkenynes*
*Hydrocarbons*
acetylenic olefinic
➤ cumulenes——see *Cumulenes*
cyclic
see
*Cycloalkadienes*
*Cycloalkenes*
➤ di-——see *Alkadienes*
exocyclic——see *Cycloalkanes, alkylidene*
perfluoro——see *Perfluorocarbons*
➤ vinyl——see *Vinyl compounds*
**waxes**——see *Paraffin waxes and Hydrocarbon waxes*
**Alkenes, properties**
double bonding in——see *Double bond*
**Alkenes, reactions**
with carbon monoxide and hydrogen——see *Hydroformylation*

**Figure 5.** Index Guide.



**Figure 6.** Hierarchy Index.

in alphabetic order, of cross-references, synonyms, and heading content notes. About 200 000 items of information are found in this collection. In addition there are four appendixes: Appendix I, Hierarchies of General Subject Headings (discussed below); Appendix II, Index to CA: Organization and Use; Appendix III, Selection of General Subject Headings; and Appendix IV, Selection of Index Names for Chemical Substances.

To demonstrate the use of the Index Guide, we will apply our question about olefins and related compounds by checking under both **Oxidation** and **Alkenes** in the Index Guide.

At the first heading (Figure 4), oxidation is defined in broad terms. Note the first statement: "Studies of oxidation. . .are indexed at this heading when the original document especially emphasizes the process or some aspect of it . . . ." We start with reaction headings such as **Oxidation** for answers to our original question because they are the important sources of the reaction information for which we are searching. Every document that reports a new reaction or a variation of an old reaction, or that in any way highlights a reaction, is indexed at a reaction heading. These reaction headings, of which there are about 290, are for the most part natural language terms that describe the changes occurring when reactants are converted to products. Such terms have accumulated over decades of indexing.

Not all natural language reaction terms, however, are valid

54. REACTION

Abstraction reaction
Addition reaction
. Acylation
. . Carbonylation
. . Carboxylation
. . Hydroformylation
. Alkenylation
. . Vinylation
. Alkylation
. . Cyanoethylation
. . Methylation
⋮
Redox reaction
. Cannizzaro reaction
. Disproportionation
. . Double decomposition
. . Redistribution reaction
. Oxidation
➤ . . Aromatization
. . Combustion
➤ . . Dehydrogenation
. . Diazotization
. . Epoxidation
. . Oxidation, aut-
. . Oxidation, electrochemical
. . . Electrolysis
. . Oxidation, photochemical
. . (Oxidative substitution)
. . . Ammoxidation
. . Oxygenation
. . Ozonization
. . Peroxidation
. Reduction
. . Birch reduction
. . Deoxidation
. . Hydrogenation
. . Hydrogenolysis
. . Methanation
. . Reduction, electrochemical
. . . Electrolysis
. . Reduction, photochemical
Reforming
⋮

**Figure 7.** Reaction hierarchy.

headings. Just prior to the beginning of the 10th Collective Period (1977–1981), the frequency with which General Subject headings for reactions were cited was examined. Those reaction headings that were cited less than 30 times during the 9th Collective Period (1972–1976) were removed and their entries were cross-referred to more general headings. As an example, **Pinacol rearrangement** had only 23 references during the 9th Collective Period. A searcher interested in current references to this reaction is directed by a cross-reference in the Index Guide to **Rearrangement**, where pinacol is given as the first word in the accompanying text. For example, the Volume 88 General Subject Index contains the entry: "Rearrangement, pinacol, in mass spectral fragmentation of alcs."

Cross-references are especially valuable when one is searching for information about named reactions. Of the more than 500 of these reactions that, at one time or another, have had headings of their own, only 36 are now indexed frequently enough to justify their own headings. The remaining named reactions are cross-referred to other headings. The Baeyer–Villiger reaction, for instance, is cross-referred to **Oxidation**, and the Gattermann aldehyde synthesis to **Formylation**.

In the Index Guide at **Oxidation**, the heading content note also indicates that "Other studies of oxidation are indexed at headings for the substances involved" (Figure 4). If oxidation is not the point of the paper and if nothing of unusual interest is disclosed, no entry will be found at **Oxidation**. For example, a paper that discusses oxidation as it is used in the conversion of one compound to another in a multistep synthesis will be cited only at the compounds involved. The text accompanying these compound entries will usually have something to say about the reaction, but no entry will be found at **Oxidation**.

42. ORGANIC COMPOUNDS

Acetals
Acids
. Arsenic acids
. Boron acids
. . Boronic acids
. . . Thioboronic acids
. . Thioborinic acids
. Carboxylic acids
. . Amino acids
⋮
Hydrazones
➤ Hydrocarbons
. Alkanes
. . Cycloalkanes
. . . Naphthenes
. . . Prismanes
➤ . Alkenes
. . Alkadienes
. . Alkenynes
➤ . . Carotenes and Carotenoids
. . Cumulenes
. . Cycloalkenes
. . . Cycloalkadienes
. . . Quinarenes
. Alkynes
⋮

**Figure 8.** Organic Compounds hierarchy.

Among the cross-references found at **Oxidation** are ones for epoxidation, ozonization, and peroxidation. For more information on these topics, we are directed to the heading for each particular topic.

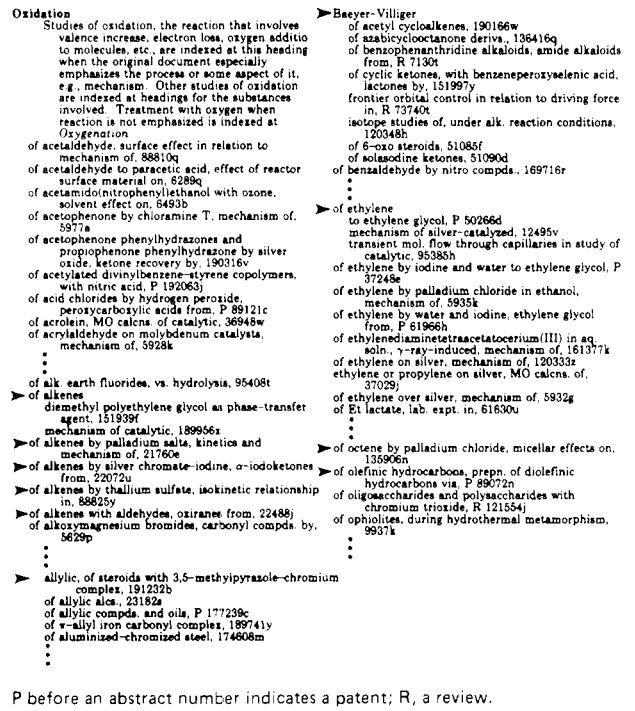
Although reaction headings are the most valuable sources of information about reactions, compound class headings can also be valuable search terms when they represent reactants or products in a new or significant reaction. Many of these classes of compounds, such as amines, alcohols, and carboxylic acids, can be found either at their own headings or cross-referenced to another heading.

We find from the Index Guide that the compound class term "olefins", used in searching the Keyword Index, is not a main heading in the General Subject Index, but is cross-referred to **Alkenes** instead. The notes in the Index Guide at **Alkenes** provide a capsule description of the indexing policies for this class of chemical compounds (Figure 5). Entries under **Alkenes** refer us to documents, reviews, books, or other broad studies in which emphasis is placed on alkenes as a class. Information at this heading also suggests several related headings, such as **Cumulenes**, **Alkadienes**, and **Vinyl compounds**, which may be added to our search profile.

**The Hierarchies of General Subject Headings.** Before proceeding to the General Subject Index, the searcher should also consult Appendix I of the Index Guide. This appendix, which contains the Hierarchies of General Subject Headings, was introduced into the Index Guide with Volume 85, published in 1977. Because the overall objective of CAS has always been to index a given subject as specifically as possible in light of the author's actual disclosure, hierarchies of headings have developed quite naturally in a number of subject areas. Both the evolution of scientific developments and the contrasts in the way that different authors have treated topics have contributed to the creation of these natural hierarchies.

The 66 subject areas that the hierarchies cover include one on reactions, with individual entries for index headings listed in order of increasing specificity. A searcher who has a specific reaction topic in mind may turn to this aid to find both more general and more specific related headings. Appendix I contains an index of these headings that refers the searcher to one or more of the hierarchies. Since almost all General Subject headings are included in these hierarchies, the index also provides a concise, alphabetic list of such headings (Figure 6).

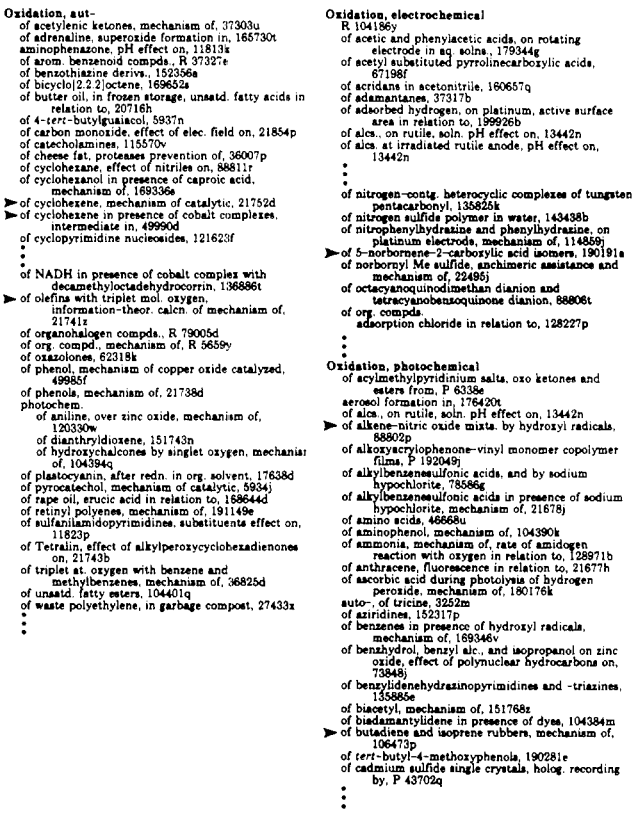
Information at **Oxidation** in the Reaction hierarchy (Figure



**Oxidation**
Studies of oxidation, the reaction that involves valence increase, electron loss, oxygen additio to molecules, etc., are indexed at this heading when the original document especially emphasizes the process or some aspect of it, e.g., mechanism. Other studies of oxidation are indexed at headings for the substances involved. Treatment with oxygen when reaction is not emphasized is indexed at *Oxygenation*.
of acetaldehyde, surface effect in relation to mechanism of, 88810q
of acetaldehyde to paracetic acid, effect of reactor surface material on, 6289q
of acetamido(nitrophenyl)ethanol with ozone, solvent effect on, 6493b
of acetophenone by chloramine T, mechanism of, 5977a
of acetophenone phenylhydrazones and propiophenone phenylhydrazone by silver oxide, ketone recovery by, 190316v
of acetylated divinylbenzene–styrene copolymers, with nitric acid, P 192063j
of acid chlorides by hydrogen peroxide, peroxycarboxylic acids from, P 89121c
of acrolein, MO calcns. of catalytic, 36948w
of acrylaldehyde on molybdenum catalysts, mechanism of, 5928k
•
•
•
of alk. earth fluorides, vs. hydrolysis, 95408t
➤ of alkenes
diemethyl polyethylene glycol as phase–transfer agent, 151939f
mechanism of catalytic, 189956x
➤ of alkenes by palladium salts, kinetics and mechanism of, 21760e
➤ of alkenes by silver chromate–iodine, α-iodoketones from, 22072u
➤ of alkenes by thallium sulfate, isokinetic relationship in, 88825y
➤ of alkenes with aldehydes, oxiranes from, 22488j
of alkoxymagnesium bromides, carbonyl compds. by, 5629p
•
•
•
➤ allylic, of steroids with 3,5–methylpyrazole–chromium complex, 191232b
of allylic alcs., 23182a
of allylic compds. and oils, P 177239c
of π-allyl iron carbonyl complex, 189741y
of aluminized–chromized steel, 174608m
•
•
•
➤ Baeyer–Villiger
of acetyl cycloalkenes, 190166w
of azabicyclooctanone derivs., 136416q
of benzophenanthridine alkaloids, amide alkaloids from, R 7130t
of cyclic ketones, with benzeneperoxyselenic acid, lactones by, 151997y
frontier orbital control in relation to driving force in, R 73740t
isotope studies of, under alk. reaction conditions, 120348h
of 6–oxo steroids, 51085f
of solasodine ketones, 51090d
of benzaldehyde by nitro compds., 169716r
•
•
•
➤ of ethylene
to ethylene glycol, P 50266d
mechanism of silver–catalyzed, 12495v
transient mol. flow through capillaries in study of catalytic, 95385h
of ethylene by iodine and water to ethylene glycol, P 37248e
of ethylene by palladium chloride in ethanol, mechanism of, 5935k
of ethylene by water and iodine, ethylene glycol from, P 61966h
of ethylenediaminetetraacetatocerium(III) in aq. soln., γ-ray–induced, mechanism of, 161377k
of ethylene on silver, mechanism of, 120332r
ethylene or propylene on silver, MO calcns. of, 37029j
of ethylene over silver, mechanism of, 5932g
of Et lactate, lab. expt. in, 61630u
•
•
•
➤ of octene by palladium chloride, micellar effects on, 135906n
➤ of olefinic hydrocarbons, prepn. of diolefinic hydrocarbons via, P 89072n
of oligosaccharides and polysaccharides with chromium trioxide, R 121554j
of ophiolites, during hydrothermal metamorphism, 9937k
•
•
•

P before an abstract number indicates a patent; R, a review.

**Figure 9.** General Subject Index.



**Oxidation, aut-**
of acetylenic ketones, mechanism of, 37303u
of adrenaline, superoxide formation in, 165730t
aminophenazone, pH effect on, 11813k
of arom. benzenoid compds., R 37327e
of benzothiazine derivs., 152356a
of bicyclo[2.2.2]octene, 169652s
of butter oil, in frozen storage, unsatd. fatty acids in relation to, 20716h
of 4-*tert*-butylguaiacol, 5937n
of carbon monoxide, effect of elec. field on, 21854p
of catecholamines, 115570v
of cheese fat, proteases prevention of, 36007p
of cyclohexane, effect of nitriles on, 88811r
of cyclohexanol in presence of caproic acid, mechanism of, 169336s
➤ of cyclohexene, mechanism of catalytic, 21752d
➤ of cyclohexene in presence of cobalt complexes, intermediate in, 49990d
of cyclopyrimidine nucleosides, 121623f
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of NADH in presence of cobalt complex with decamethyloctadehydrocorrin, 136886t
➤ of olefins with triplet mol. oxygen, information–theor. calcn. of mechanism of, 21741s
of organohalogen compds., R 79005d
of org. compd., mechanism of, R 5659y
of oxazolones, 62318k
of phenol, mechanism of copper oxide catalyzed, 49985f
of phenols, mechanism of, 21738d
photochem.
of aniline, over zinc oxide, mechanism of, 120330w
of dianthryldioxene, 151743n
of hydroxychalcones by singlet oxygen, mechanism of, 104394q
of plastocyanin, after redn. in org. solvent, 17638d
of pyrocatechol, mechanism of catalytic, 5934j
of rape oil, erucic acid in relation to, 168644d
of retinyl polyenes, mechanism of, 191149e
of sulfanilamidopyrimidines, substituents effect on, 11823p
of Tetralin, effect of alkylperoxycyclohexadienones on, 21743b
of triplet at. oxygen with benzene and methylbenzenes, mechanism of, 36825d
of unsatd. fatty esters, 104401q
of waste polyethylene, in garbage compost, 27433x
•
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**Oxidation, electrochemical**
R 104196y
of acetic and phenylacetic acids, on rotating electrode in aq. solns., 179344g
of acetyl substituted pyrrolinecarboxylic acids, 67198f
of acridans in acetonitrile, 160657q
of adamantanes, 37317b
of adsorbed hydrogen, on platinum, active surface area in relation to, 199926b
of alcs., on rutile, soln. pH effect on, 13442n
of alcs. at irradiated rutile anode, pH effect on, 13442n
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•
•
of nitrogen–contg. heterocyclic complexes of tungsten pentacarbonyl, 135825k
of nitrogen sulfide polymer in water, 143438b
of nitrophenylhydrazine and phenylhydrazine, on platinum electrode, mechanism of, 114859j
➤ of 5–norbornene–2–carboxylic acid isomers, 190191a
of norbornyl Me sulfide, anchimeric assistance and mechanism of, 22495j
of octacyanoquinodimethan dianion and tetracyanobenzoquinone dianion, 88806t
of org. compds.
adsorption chloride in relation to, 128227p
•
•
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**Oxidation, photochemical**
of acylmethylpyridinium salts, oxo ketones and esters from, P 6338e
aerosol formation in, 176420t
of alcs., on rutile, soln. pH effect on, 13442n
➤ of alkene–nitric oxide mixts. by hydroxyl radicals, 88802p
of alkoxyacrylophenone–vinyl monomer copolymer films, P 192049j
of alkylbenzenesulfonic acids, and by sodium hypochlorite, 78586g
of alkylbenzenesulfonic acids in presence of sodium hypochlorite, mechanism of, 21678j
of amino acids, 46868u
of aminophenol, mechanism of, 104390k
of ammonia, mechanism of, rate of amidogen reaction with oxygen in relation to, 128971b
of anthracene, fluorescence in relation to, 21677h
of ascorbic acid during photolysis of hydrogen peroxide, mechanism of, 180176k
auto–, of tricine, 3252m
of aziridines, 152317p
of benzenes in presence of hydroxyl radicals, mechanism of, 169346v
of benzhydrol, benzyl alc., and isopropanol on zinc oxide, effect of polynuclear hydrocarbons on, 73848j
of benzylidenehydrazinopyrimidines and -triazines, 135885e
of biacetyl, mechanism of, 151768z
of biadamantylidene in presence of dyes, 104384m
➤ of butadiene and isoprene rubbers, mechanism of, 106473p
of *tert*-butyl-4-methoxyphenols, 190281e
of cadmium sulfide single crystals, holog. recording by, P 43702q
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**Figure 10.** General Subject Index.

7) partially duplicates information found in the main part of the Index Guide. It also makes clear, however, that reactions such as aromatization and dehydrogenation are specific examples of oxidation. To locate information on these topics, we would have to frame our search questions in terms of these more specific topics in addition to checking the more general headings.

The Organic Compounds hierarchy (Figure 8) lists **Alkenes** as a heading. It is shown to be a subgroup of **Hydrocarbons** and in turn is the more general term for **Carotenes and Carotenoids**, adding another potential search term. By checking these headings for related entries we can come a step closer to feeling that we have found all relevant references to our search topic.

**The General Subject Index.** Having consulted the Index Guide for relevant search headings, we are ready to consult the Volume Indexes. Although there are several types of Volume Indexes, for the purposes of our question we will mainly consider the General Subject Index. The **Oxidation** heading in the General Subject Index contains the same heading content notes as those that defined the scope of the headings in the Index Guide (Figure 9). The entries consist primarily of many columns of text which include the words and phrases that accompany the headings, and the corresponding abstract numbers. From the information contained in this text, the searcher decides whether to consult the abstract.

The text of the General Subject Index is written to give the most important information first. At reaction headings, such as **Oxidation**, this information may be the specific substrate acted upon, such as ethylene or octene, or a class of compounds such as alkenes. It may be a specific oxidation that is not indexed at its own heading, such as allylic, or a named oxidation that does not justify a heading of its own, such as Baeyer–Villiger. Some standardization and vocabulary control have been imposed on the initial information, but the text is generally freely written, reflecting the emphasis and terminology of the original document. For a complete search under any index heading, this fact should be kept in mind.

To continue our search for information about olefins and related compounds under **Oxidation**, we would search the text for the compound class words, alkenes and olefins, that we selected earlier in our search. We must also examine the entire listing, however, because some key words and phrases may be embedded in the text.

In addition to the so-called plain heading, **Oxidation**, there are three other oxidation headings that we need to consider in our search: **Oxidation, aut-**; **Oxidation, electrochemical**; and **Oxidation, photochemical** (Figure 10). We should also consult the entries under the catalyst headings, such as **Oxidation catalysts**, and under **Kinetics of oxidation** and **Heat of oxidation**, to find further information (Figure 11).

When we turn to **Alkenes** in the General Subject Index we find that the heading itself is subdivided into a number of separate headings. Since 1967, large headings such as this have been divided into seven subdivisions to simplify searching. The seven subdivisions are analysis, biological studies, occurrence, preparation, properties, reactions, and uses and miscellaneous. The one that interests us at present is reactions (Figure 12).

At the reactions subdivision of **Alkenes** we find many entries at the opening phrase "oxidn. of" with, expectedly, some overlap with the entries found at **Oxidation**. Looking at other entries we find, for example, "autoxidn. of" and "epoxidn. of", which may also give us information relevant to our search. We could continue by looking at **Dehydrogenation**, **Epoxidation**, **Peroxidation**, and other related reaction headings; at **Alkadienes**, **Cumulenes**, **Vinyl compounds**, and at other classes of compound headings; and at specific alkenes such as ethene and 1-propene, which are found in the Chemical Substance Index. All of these headings are suggested by entries either in the main body of the Index Guide or in the Hierarchies of General Subject Headings at **Reactions** or **Organic Compounds**.

The examples we have discussed illustrate how a searcher would use CAS publications and services to answer a fairly general question concerning a reaction. The searcher would

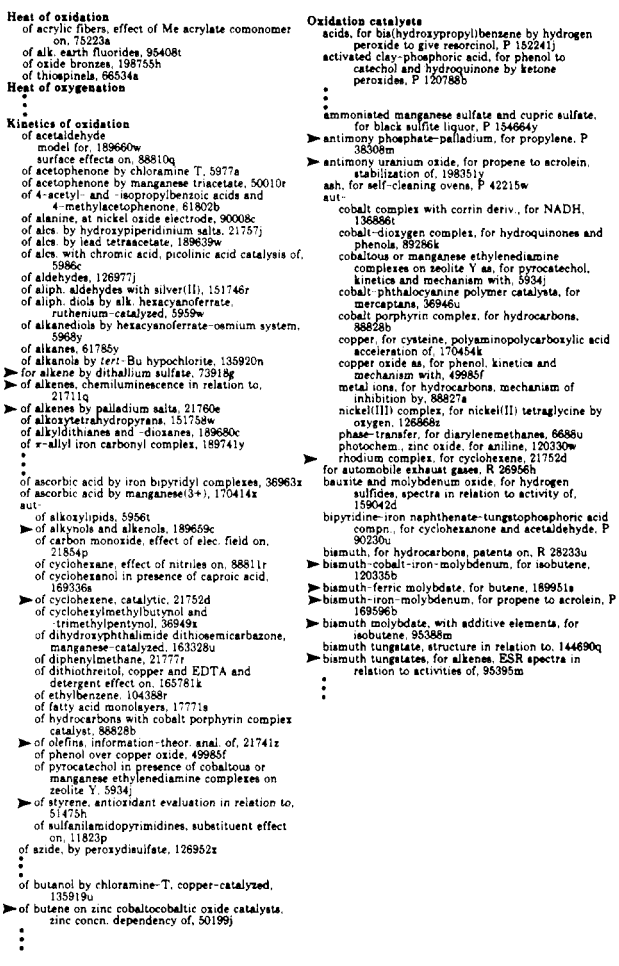


Figure 11. General Subject Index.

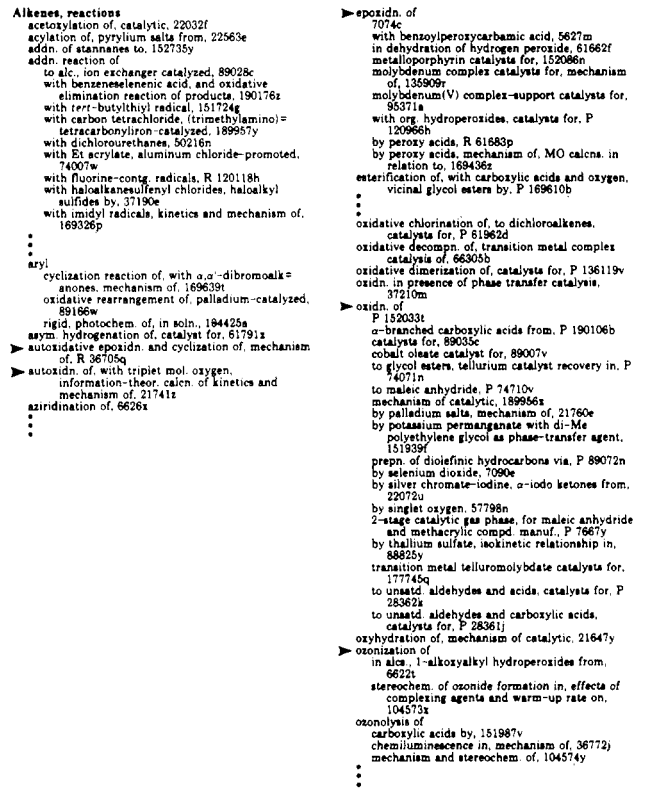


Figure 12. General Subject Index.

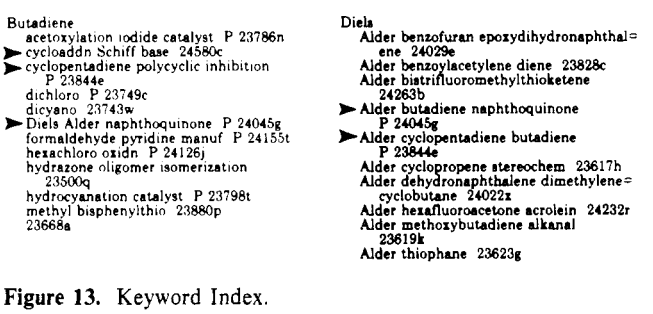


Figure 13. Keyword Index.

**1,3-Butadiene** (*bivinyl*) [*106-99-0*]
Studies of "butadiene" are indexed at this heading
in the absence of further information

Figure 14. Index Guide.

begin by phrasing the search question carefully. Next, he or she would consult the Keyword Index contained in each issue of CA for search terms related to the question. To find additional search terms, the searcher could also consult the CA Condensates Search Aid Package, and particularly its KLIC Index.

The Index Guide will supply search terms and direct the searcher to appropriate headings in the Volume Indexes. A searcher could obtain more specific or more general terms from the Hierarchies of General Subject Headings. Finally, the searcher would consult the entries under these terms in the Volume Indexes to determine which abstracts to search. The answer, of course, will consist only of abstract numbers. Completion of the search would require the searcher to read the abstracts, and then the original documents for those references that seem most relevant.

## SEARCHING FOR INFORMATION USING A SPECIFIC SEARCH QUESTION

Our first search problem, "What new information has been published recently about the oxidation of olefins and related compounds?", was a very general and a very difficult one. A relatively large number of search terms were used as keys to different CA Indexes, many entries were scanned, and references to a large number of documents were retrieved. From these, we then selected entries related to our purposes.

In contrast, by restricting the search to a more specific problem, the search becomes easier in many ways and yields more complete results. A specific search problem is illustrated by the second or our two search questions: "What new information concerning the Diels–Alder reaction of butadiene is available?".

For a search of the most recent literature, the Keyword Index is addressed at "Butadiene" and at "Diels–Alder". In a recent issue, the relevant entries shown in Figure 13 are found. Other search terms that might be used by an author, such as cycloaddition, must also be considered. Since the search problem is relatively restricted, small numbers of references will be found.

It is worth pointing out that, in general, the reactant and the reaction will be found in one Keyword Index entry, and the product of the reaction in a separate entry. This policy restricts the number of words in any one entry, allows rapid scanning, relates a reactant to its reaction, and permits access to information by a number of entry points.

For a retrospective search of the question, the simplest and most complete procedure will be through the Chemical Substance Index, by way of the Index Guide. All reactants, as well as intermediates and products, are indexed, and thus

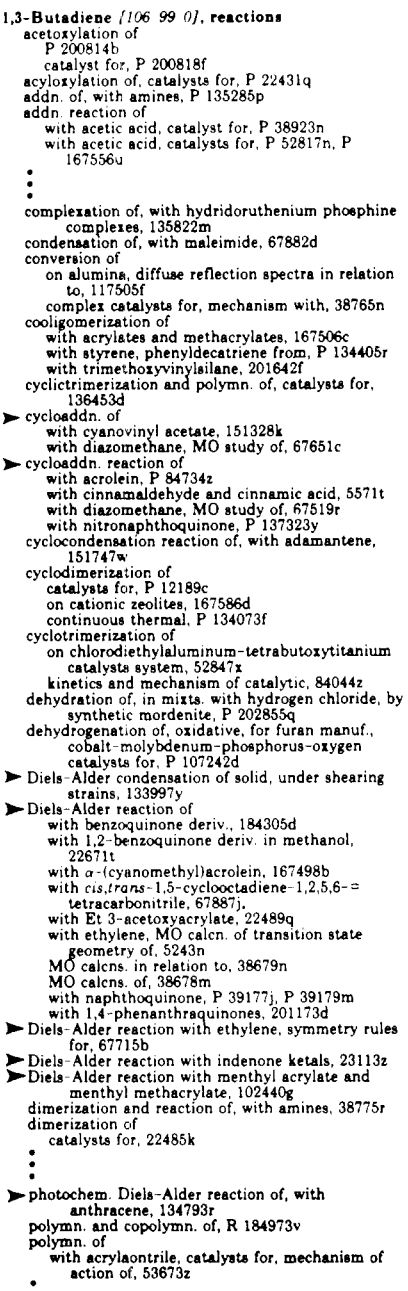


**Figure 15.** Chemical Substance Index.

all reactions of butadiene will be found in the Chemical Substance Index. As the Index Guide points out, studies of

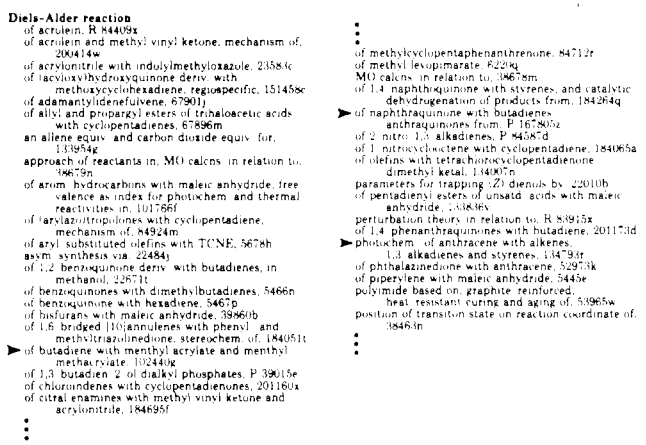


**Figure 16.** General Subject Index.

butadiene are indexed at the 1,3 isomer (Figure 14).

Butadiene is one of the most frequently cited organic substances. For ease of information retrieval, it, like the class heading **Alkenes**, is subdivided. Diels–Alder reactions of butadiene will, of course, be found in the reactions subdivison. Examination of the Volume 87 Chemical Substance Index shows many pertinent entries, some of which are shown in Figure 15.

Again note the free-form construction of the text. Most of the entries of interest are listed at "Diels–Alder reaction of", but one entry is located at "photochem. Diels–Alder reaction of" and another at "cycloaddn. reaction of". This is the result of the use of author terminology; there is no requirement that a standard reaction term be used in the text.

Significant studies of the Diels–Alder reaction will be found in the General Subject Index at **Diels–Alder reaction** (Figure 16). It is obvious that the most relevant references to the Diels–Alder reaction of butadiene will be those in which both the reaction and the reactant are indexed. Less relevant references will be found only at **1,3-Butadiene**, but even these may merit examination.

## SUMMARY

In summary, to find current information about reactions, the searcher looks at the Keyword Index in the abstract issues for terms describing the reactions and reactants. The searcher uses the language found in the literature, as well as the entries in the KLIC Index, to find related terms.

For retrospective searches, the searcher must consult the Index Guide as the key to the Volume Indexes. Using CA-preferred terminology, the searcher then uses the Chemical Substance Index to obtain information about reactants, intermediates, and products, and the General Subject Index for information on reactions and compound classes.