

- (11) Speck, P. T. "Übersetzung von Linien- und Flächenstrukturen in kombinatorisch-relationale Datenstrukturen zur automatischen Mustererkennung in Digitalbildern". Dissertation 7508, ETH Zürich, 1984.
- (12) Danielsson, P. E. "An Improved Segmentation and Coding Algorithm for Binary and Nonbinary Images". *IBM J. Res. Develop.* 1982, 26, 698-707.
- (13) Ramachandran, K. "Coding Method for Vector Representation of Engineering Drawings". *Proc. IEEE* 1980, 68, 813-817.
- (14) "Status Report of the Graphic Standards Planning Committee". *Comput. Gr.* 1979, 13.
- (15) Enderly, G.; Kansy, K.; Pfaff, G. "Computer Graphics Programming. GKS—the Graphic Standard"; Springer: Berlin, 1984.

The Chemical Reactions Documentation Service: Ten Years On†

ALAN F. FINCH

Derwent Publications Ltd., Rochdale House, London WC1X 8RP, England

Received August 12, 1985

The philosophical basis, historical development, and essential features of Derwent's Chemical Reactions Documentation Service are outlined with particular reference to the monthly *Journal of Synthetic Methods*, the link with Theilheimer's *Synthetic Methods of Organic Chemistry*, and the two computer-based systems used for retrieval.

During the last 4 decades, William Theilheimer's annual volumes of *Synthetic Methods of Organic Chemistry*¹ have afforded the practicing chemist direct and comprehensive access to the key organic reactions reported in the literature. With the active support of a team of technical advisors in Europe and the U.S., the editor of this renowned series guided the first 35 volumes through a period when synthetic chemistry underwent radical change and development. On Theilheimer's retirement in 1981, the responsibility for producing the yearbooks was passed to Derwent Publications Ltd., which some 5 years earlier had introduced the monthly *Journal of Synthetic Methods* (JSM)² as an adaptation of the yearly volumes. Today JSM provides the input for *Synthetic Methods* and is at the same time the cornerstone of Derwent's Chemical Reactions Documentation Service (CRDS). In this paper, the philosophical basis, the historical development, and essential features of this service are described with an illustration of retrieval capabilities from the current database of over 60 000 reactions.

PHILOSOPHY, SCOPE, AND COORDINATION

The growth of the scientific literature should ideally be matched by the development of efficient means of accessing the information contained therein. For retrieval of specific compounds and compound classes, this has been largely the case. For chemical reactions, however, the development of retrieval methods progressed more slowly, and it was not until Theilheimer came on the scene that a comprehensive and analytical system for collating, indexing, and presenting synthetic methods became available. That this system and the philosophy behind *Synthetic Methods* have remained basically unchanged through the years is validation in itself, and with current refinements, computer-based equivalents, and extensions in JSM, it is enjoying a new lease of life and recognition.

For both JSM and *Synthetic Methods*, selection of material is still the most critical phase, as may be appreciated from the crude representation of the chemical literature as shown in Figure 1. In this analogy with an "inverted iceberg", the bulk of synthetic organic chemistry—pertaining largely to applications of known methods and specialized fields of chemistry—is clear to view and readily accessible by conventional retrieval techniques and handbooks. Much less so,

however, are the data beneath the surface: namely, the 2000–3000 new synthetic methods published each year, plus—in the darkened area—approximately the same number of additional publications describing minor modifications of known methods. It is the material in these two lower layers that is presented in JSM: the former as informative abstracts on such aspects as novel functional group and ring transformations of a general nature, new reagents and synthetic techniques, and new syntheses of key ring systems; and the minor modifications as additional data published biannually in *Supplementary Reference Indexes*.

Reactions are selected for JSM by scrutiny of the worldwide journal and patents literature and are usually published some 6–8 weeks from receipt of the primary documents. The novelty of the data is confirmed by a prior analysis, or coordination, with the current CRDS database, which comprises over 60 000 key reactions from *Synthetic Methods* Volumes 1–30 (containing information from 1942 to 1975) and JSM itself (1975 to date). Such coordination is also necessary in order to identify the original methods to which to append the supplementary references. In this way, key synthetic items are located quickly and available in a compact form ideal in size to allow rapid scanning on a monthly basis and with cumulated subject indexes for retrospective searching.

FORMAT OF THE JOURNAL OF SYNTHETIC METHODS

The structure of the journal is similar to that developed by Theilheimer for *Synthetic Methods*. The abstracts, illustrated in Figure 2, feature a Derwent-assigned title, a typical experimental procedure, and, most important for scanning purposes, a clearly expressed reaction scheme. The reactions, numbering 250 in each monthly issue, are arranged according to Theilheimer's **reaction symbol notation**, the systematic classification given at the top of the abstract, so that all the reactions of a given type are found together.

The entries in the *Subject Indexes* (Figure 3) include starting materials, products, reagents, and any other synthetic items considered relevant. Where appropriate, a dynamic term, such as C-alkylation, may be used but the indexing normally takes the form "A starting material for B" and "B from A". Systematic nomenclature is used throughout and supported by a unique cross-reference network, so critical for comprehensive retrieval. This comprises three essential elements: synonyms, cross-referencing to related concepts, and

† Presented at the 188th National Meeting of the American Chemical Society, Philadelphia, PA, Aug 30, 1984.

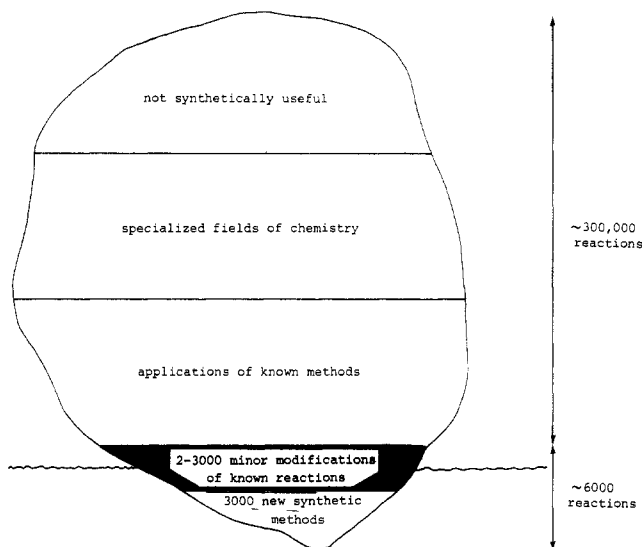


Figure 1. Representation of the number and nature of organic reactions published each year in the literature.

the "special sec" subdivision, the latter directing the reader to the nomenclature of complex functions via that of the constituent residues. This is illustrated in Figure 4 for the functional group $RS-C-S(O)R'$, for which the subject index nomenclature is **1-Sulfinylthioethers**.

The *Formula Index of Complex Functional Groups* was designed as an independent means of locating the functional group nomenclature. This comprises a listing of functional groups in terms of the essential (invariant) elements, not unlike the molecular formula for specific compounds. The function $RS-C-S(O)R'$, for example, reduces to the formula OS_2C , as can be seen in Figure 5 with the associated nomenclature of this and other functional groups with the same formula.³

The 2000–3000 supplementary reactions, represented as the darkened area in Figure 1, are minor modifications of known methods previously abstracted in either *Synthetic Methods* or JSM. Included in this number are some 1000 catalytic processes reported every year in the patents literature, such

as the olefin conversions shown in Figure 6. While novelty there may be in respect of catalytical modification, it is not JSM policy to present the information as abstracts, which would considerably dilute the main file. Rather, they are indexed in the biannual *Supplementary Reference Indexes*, as illustrated in Figure 7. Access to the original abstract numbers to which the supplementaries are appended is either via the *Subject Indexes* or by the computer-based systems described below, either route leading to updated information on established reactions twice each year.

The two remaining features of JSM are the Reviews page and the Highlights page, both prominent at the front of each issue and used as the basis of the **Trends** in *Synthetic Methods*.

COMPUTER-BASED RETRIEVAL SYSTEMS

While access to most scientific data can be gained through subject indexes, the questions of speed and convenience naturally become important as the volume of data expands. For the CRDS file, two independent computer-based retrieval systems are available: the Coding and the Keywording. The former was initially designed for in-house use, but is also available online through public telephone access to a central computer; the more recent Keywording is available only online.⁴ The main features of these two systems are outlined below.

THE CODING SYSTEM

This, the earlier of the two retrieval systems, was developed in the late 1960s by the Pharma Dokumentationsring, a consortium of mainly European pharmaceutical companies, and originally designed for in-house retrieval of the reactions in *Synthetic Methods*. Originally based on the 80-column IBM punch card, it is a formal system by which the key reaction parameters—starting materials, products, reagents, bond breakages and formations, and reaction conditions—are input and retrievable as three-digit codes.

Considering, for example, the reduction of azido to amino groups, the search strategy would simply be a combination of six numbers, as seen in Figure 8. Thirty-six references resulted

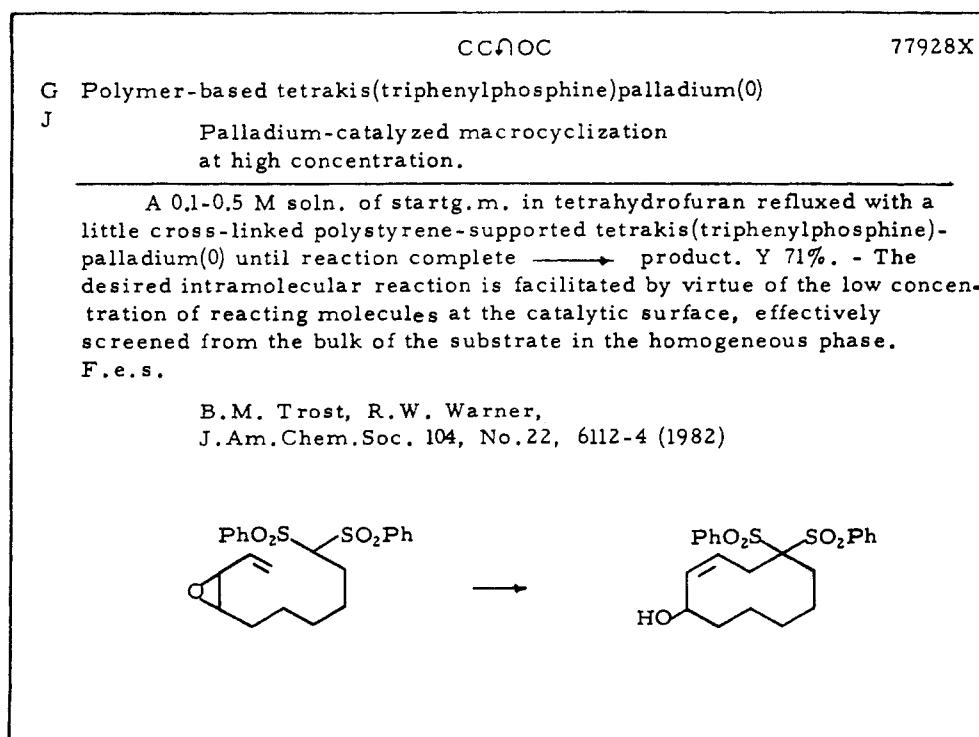


Figure 2. Sample abstract in the *Journal of Synthetic Methods*.

:
o-Acylation
 - of
 phenols 5960

Acylcyanamides
 - startg.m.f.
 4(4H)-1,3-oxazinones,2-
 acylamino- 5808

Acylhydrazines
 - startg.m.f.
 2(1H)-pyridones,1-amino-,
 polysubst. 5907

N-Acyl- α -ketocarboxylic
 acid amides
 - from
 2-pyrazinone-3,6-
 endoperoxides 5796

Acyl peroxides
 - special s.
 bis(heptafluorobutyl)
 peroxide

Acylsilanes
 - special s.
 α,β -ethyleneacylsilanes

 α -Acylthiocarboxylic acid
 esters
 - startg.m.f.
 β -ketocarboxylic acid
 esters 5994

N-Acylthionylimines
 - startg.m.f.
 1,4,3-oxathiazine 4-
 oxides,5,6-dihydro-
 5874

1,4-Addition 5914, 5916
1,4-Addition,asym. 5912
 :

Figure 3. Section of Subject Index.

:
Meraptal mono-S-oxides s. 1-Sulfinylthioethers
 :
 → 1-Sulfinylthioethers
 :
Sulfoxides (s.a. Sulfinyl...)
 :
Thioethers
 - special s.
 1-sulfinylthioethers
 :

Figure 4. Illustration of the cross-reference network of the Subject Index.

from the online interrogation of the complete CRDS database (>60 000 reactions) from 1942 to 1984, the printout for the eight most recent references being given in Figure 9. The relevance of the search can readily be assessed by inspection of the corresponding reaction symbol notation, $\text{HN}\downarrow\text{N}$ (online as HN-X-N), which is printed out after the title. Details of the Coding system have been published elsewhere.⁵

THE KEYWORDING SYSTEM

The second method for retrieval, the Keywording, was introduced in 1978 and was specifically designed to take advantage of the facilities offered by online retrieval.

:
OS₂
 Disulfide monoxides
 Thiosulfinyl esters
 Thiolsulfinates

OS₂C
 Acyl disulfides
 Dithiolcarbonic acid esters
 Dithiolortholactones
 1-Organothiosulfinates
 → 1-Sulfinylthioethers
 Xanthates
 Dithiocarbonic acid O,S-
 diesters

OS₂C₂
 Acyl thioacyl sulfides
 1-Alkylthiothiolic acid esters
 1-Sulfinylthioenolethers

OS₂C₃
 Acylene-1,1-dithiols
 α -Ketoketene mercaptals
 α -Dimercaptomethyleneketones
 :

Figure 5. Section of the Formula Index of Complex Functional Groups.

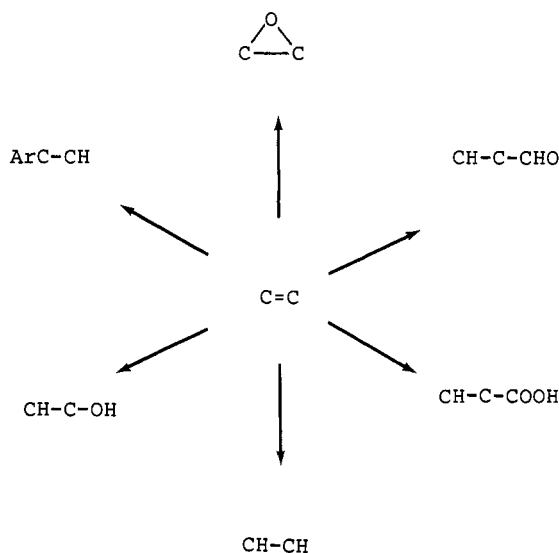
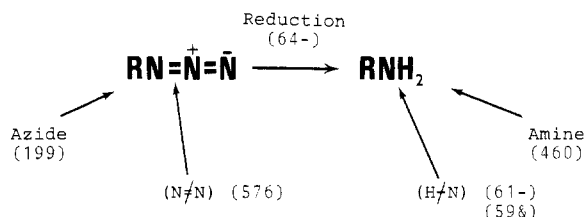


Figure 6. Typical catalytic processes from patents literature.

:
 77108R cf. US-4411905 (83-814602)
 77131R s.a. J5-9020424 (84-065046); DE-3220729 (83-839437)
 77183R s.a. Tetrahedron 19, No.6, 975-82 (1983)
 77185R dimerization of ethylenes s.a. J5-8146517 (83-785451); J5-8146518 (83-785452);
 FR-2524341 (83-809750); SU-1004331 (84-016373); EP-91232 (83-790356);
 J5-8180434 (83-829932)
 77188R hydroformylation (cf. 4,667) s.a. EP-89697 (83-778413); DD-204241 (84-069504);
 EP-94748 (83-828485); DE-3220858 (83-839506); J5-8186443 (83-836429);
 US-4417077 (83-838890); BE-897966 (84-049518); SU-994461 (83-831927);
 EP-96987 (84-001352); EP-96988 (84-001353); J5-8205549 (84-013801);
 US-4432904 (84-062553); US-435517 (84-074891); J5-8180236 (83-829886);
 EP-96986 (84-001351); J5-8201743 (84-007972); EP-89690 (83-778406);
 US-4413146 (83-820498); EP-94456 (83-828267); J5-9020238 (84-065044);
 DD-204242 (84-069505); review of hydroformylation of unsaturated fatty acids s.
 J.Am.Oil Chem.Soc. 61, No.2, 419-25 (1984)
 77189R carbonylation s.a. J5-8214345 (84-021784); J5-9010545 (84-052401); EP-95431
 (83-834650); US-4414409 (83-826759); DE-3213395 (83-789751); J5-8198441
 (84-002886); SU-559548 (84-054059); EP-92491 (83-803014); asym.
 carbonylation s. J5-8167541 (84-020053)
 :

Figure 7. Section of Supplementary Reference Index.

Strategy:

SS 1 /C?
 USER:
 199 AND 576 AND 61- AND 460 AND 59& AND 64-

Figure 8. Example of a search strategy using the Coding.

```

SS 1 /C?
USER:
199 AND 576 AND 61- AND 460 AND 59& AND 64-

SS 1 PSTG (36)

SS 2 /C?
USER:
PRT 8

PROG:

-1-
AN - 77509Z RY
TI - /AMINES FROM AZIDES UNDER MILD CONDITIONS . SELECTIVE REDUCTION/
    HN-X-N //
CI - CHEM.LETTERS 1984, NO.10, 1733-6.

-2-
AN - 77760Y R
TI - /AZETIDINES FROM 2-AZETIDINONES/ HC-X-O //
CI - J.AM.CHEM.SOC. 105, NO.20, 6339-42 (1983).

-3-
AN - 76252Y R
TI - /AMINES FROM AZIDES . TRANSFER HYDROGENATION/ HN-X-N //
CI - TETRAHEDRON LETTERS 24, NO.15, 1609-10 (1983).

-4-
AN - 77508X R
TI - /AMINES FROM AZIDES/ HN-X-N //
CI - CHEM.IND. 1982, NO.18, 720.

-5-
AN - 77507X R
TI - /AMINES FROM AZIDES . PHASE TRANSFER CATALYSIS/ HN-X-N //
CI - J.ORG.CHEM. 47, NO.22, 4327-9 (1982).

-6-
AN - 76101W R
TI - /CYCLIC AMIDINES FROM IMINOHALIDES VIA IMINOAZIDES .
    4-AMINOPYRIMIDINES/ NC-X-G, HN-X-N //
CI - J.ORG.CHEM. 46, NO.7, 1413-23 (1981).

-7-
AN - 75503W R
TI - /AMINES FROM AZIDES UNDER NEUTRAL CONDITIONS . SELECTIVE
    REDUCTION . AR. AMINES/ HN-X-N //
CI - J.CHEM.RES.(S) 1981, NO.1, 17.

-8-
AN - 77753V R
TI - /AMINES FROM AZIDES . HETEROCYCLIC PRIM . AMINES . ALSO FROM
    HYDRAZINES/ HN-X-N //
CI - SYNTHESIS 1980, NO.10, 830-31.
  
```

Figure 9. Printout of the first eight references corresponding to the search strategy given in Figure 8.

A controlled keyword list was developed, comprising some 1000 terms for starting materials and products and around 700 terms for generic reagent classes, reaction conditions, and reaction types. Where possible, nomenclature is such as to permit retrieval of related keywords in a single operation by right-hand truncation. Thus, all selenium and silicon keywords shown in Figure 10 are retrievable with the truncated fragments SE and SI, respectively.

Included in the keyword list for starting materials and products are around 250 terms for ring systems, such as DIOXOLE-1,2 and DIOXOLE-1,3 and a number of **structural keywords**—a novel indexing feature that adds a degree of chemical integrity to an otherwise formal system. With these one can locate substructure fragments of a general nature, such as $-\text{O}-\text{C}-\text{N}-$, $-\text{O}-\text{C}-\text{C}-\text{O}-$, $-\text{N}-\text{C}-\text{C}(=\text{Y})-$, and thereby perform broad searches without specifying the exact nature of the groups involved; e.g., the structural keyword DIOXY-1,2 (for the fragment $-\text{O}-\text{C}-\text{C}-\text{O}-$) will recall all

```

:
DIOL
DIOXIN-1,2
DIOXIN-1,3
DIOXIN-1,4
DIOXO-COMPD
DIOXOLE-1,2
DIOXOLE-1,3
DIOXY
DIOXY-1,1
DIOXY-1,2
DIOXY-1,3
:
SELENIDE
SELENIDE+
SELENIDE,AR
SELENIDE,CYCLIC
SELENIUM
SELENOL
:
:
SELENOL,AR
SELENOXIDE
SELENYLHALIDE
SI-ACID
SI-AMINE
SI-AMIDE
SI-ETHER
SI-ETHER+
SI-HALIDE
SI-HYDRIDE
SI-THIOACID
SI-THIOETHER
SI-THIOETHER+
SILANE
SILANE+
SILICIC
SILICON
SILYL
SILYL,TRIMETHYL
:
:
  
```

Figure 10. Sections of the Keyword list.

TG	Application
A	Aromatic substitution and exchange Aromatization and dearomatization Aromatic ring opening (in addition to I) Aromatic ring closure (in addition to J)
B	Biochemical reaction
C	Carbohydrate chemistry
E	Electrochemical reaction
G	Heterocyclic ring opening
H	Heterocyclic ring closure
I	Isocyclic ring opening
J	Isocyclic ring closure
K	Ring contraction
L	Ring expansion
:	:
:	:

Figure 11. Some examples of thematic groups with definitions.

glycols ($\text{HO}-\text{C}-\text{C}-\text{OH}$) and their derivatives ($\text{RO}-\text{C}-\text{C}-\text{OH}$, and $\text{RO}-\text{C}-\text{C}-\text{OR}$, $\text{RSO}_2\text{O}-\text{C}-\text{C}-\text{OSO}_2\text{R}$, etc.) in one operation. A limited number of **adjectival keywords**, e.g., DI-HYDRO, TETRAHYDRO, UNSATD, is also available for refining searches, as illustrated below for the retrieval of pyrans and hydrogenated pyrans:

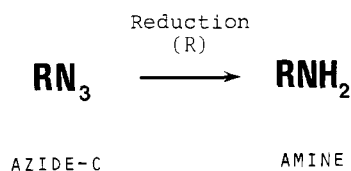
PYRAN retrieves all pyrans
 (unsaturated and hydrogenated)

PYRAN AND DIHYDRO retrieves all dihydropyrans

PYRAN AND TETRAHYDRO
 retrieves all tetrahydropyrans

PYRAN AND UNSATD retrieves all unsaturated pyrans

Broad reaction concepts, such as reduction, oxidation, rearrangement, electrolysis, and protective group chemistry, are retrievable by single-letter reactions classes (**thematic groups**) some of which are given in Figure 11. These may be supplemented by **reaction keywords** for greater specificity. Thus, while the letter Z retrieves all protective group chemistry, the reaction keywords PROTECTION-OH and PROTECTION-NH may be used for locating all papers on (de)protection of hydroxyl and amino groups, respectively. Specific reagents are retrievable by using standardized *Synthetic Methods* nomenclature, e.g., CUPROUS-CHLORIDE and TRI-ETHYLAMINE, whereas a controlled list of generic reagent keywords is available for retrieval of classes of reagent, e.g.,

Strategy:

SS 1 /C?
 USER:
 AZIDE-C/SM AND AMINE/PR AND R/TG

Figure 12. Example of a search strategy using the Keywording.

```

SS 1 /C?
USER:
AZIDE-C/SM AND AMINE/PR AND R/TG

SS 1 PSTG (19)

SS 2 /C?
USER:
PRT 7

PROG:

-1-
AN - 77509Z RY
TI - /AMINES FROM AZIDES UNDER MILD CONDITIONS . SELECTIVE REDUCTION/
HN-X-N / /
CI - CHEM. LETTERS 1984, NO.10, 1733-6.

-2-
AN - 76252Y R
TI - /AMINES FROM AZIDES . TRANSFER HYDROGENATION/ HN-X-N / /
CI - TETRAHEDRON LETTERS 24, NO.15, 1609-10 (1983).

-3-
AN - 77508X R
TI - /AMINES FROM AZIDES/ HN-X-N / /
CI - CHEM. IND. 1982, NO.18, 720.

-4-
AN - 77507X R
TI - /AMINES FROM AZIDES . PHASE TRANSFER CATALYSIS/ HN-X-N / /
CI - J. ORG. CHEM. 47, NO.22, 4327-9 (1982).

-5-
AN - 77503W R
TI - /AMINES FROM AZIDES UNDER NEUTRAL CONDITIONS . SELECTIVE
REDUCTION . AR. AMINES/ HN-X-N / /
CI - J. CHEM. RES. (S) 1981, NO.1, 17.

-6-
AN - 77753V R
TI - /AMINES FROM AZIDES . HETEROCYCLIC PRIM . AMINES . ALSO FROM
HYDRAZINES/ HN-X-N / /
CI - SYNTHESIS 1980, NO.10, 830-31.

-7-
AN - 76760V GR
TI - /REDUCTIVE RING OPENING OF 3-SUBST . 2-AZETIDINONES . ALPHA-
AMINOCARBOXYLIC ACID AMIDES FROM 3-AZIDO-2-AZETIDINONES . ALPHA-
HYDROXYCARBOXYLIC ACID AMIDES FROM 3-BENZYLOXY-2-AZETIDINONES, AND
OPTICALLY ACTIVE COMPS/ HC-X-N, HC-X-C / /
CI - CHEM. LETTERS 1980, NO.7, 853-56.
  
```

Figure 13. Printout of the first seven references corresponding to the search strategy given in Figure 12.

CU-1 for all copper(I) compounds and AMINE, TERT for all tertiary amines.

In order to define the role of keywords—as starting materials, products, reagents, etc.—the following search qualifiers are available:

- /SM for starting materials
- /PR for products
- /RT for reagents and reaction terms
- /TG for thematic groups

These are suffixed to the appropriate keywords, which may then be combined in a search by using Boolean operators. This is exemplified in Figure 12 for the reduction of aliphatic azides to amines, the printout (Figure 13) showing the seven most recent references. By comparison with the Coding search (Figures 8 and 9), the response is lower, partly because the latter was a general search for all amines (aliphatic, aromatic, heterocyclic) and partly because a smaller file was searched (1966–1984). For reduction of aromatic azides, for example, the keyword search strategy would have AMINE, AR/PR in

```

SS 3 /C?
USER:
PRT AN TI CI KW 1

PROG:

-1-
AN - 77509Z RY
TI - /AMINES FROM AZIDES UNDER MILD CONDITIONS . SELECTIVE REDUCTION/
HN-X-N / /
CI - CHEM. LETTERS 1984, NO.10, 1733-6.
KW - /AZIDE-C/ GIVES *AMINE, AR* *AMINE* INORG-REDN TE
(SODIUM-HYDROGEN-TELLURIDE) SOLV=4 TEMP=4 *(KETONE)* *(ETHYLENE)*
*(ACETYLENE)* *(C-ACID)* *(C-AMIDE)* *(C-ESTER)* *(NITRILE)*
*(HALIDE, AR)* *(HALIDE)* *(SULFONE)*
  
```

Figure 14. Sample Keywording record in full.

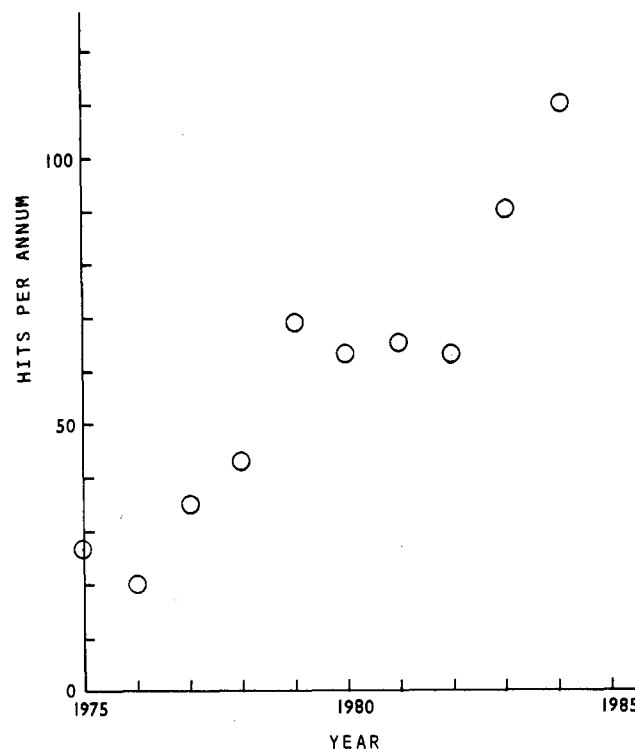


Figure 15. Graphical representation of a search for asymmetric synthesis covering the period 1975–1984 (30 000 reactions).

place of AMINE/PR, while the strategy for reduction of both aliphatic and aromatic azides would be

AZIDE-C/SM AND R/TG AND ALL AMINE/PR

The full printout of the first answer on the list, abstract 77509Z, is shown in Figure 14. Of special note are the keywords enclosed by both asterisks and parentheses, e.g., *(KETONE)*, which illustrates the indexing of an unaffected function. For retrieval of the latter, the keyword is searched in the following manner:

'KETONE' /PR

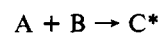
Thus, one could retrieve all reductions that leave keto groups unaffected by the following strategy:

R/TG AND 'KETONE' /PR

This aspect of "negative" indexing and retrieval is also used in the keywording of activating groups, such as the keto group in the α -halogenation of ketones.

Trends in synthesis over a particular period may be discerned from keyword searches on specific subjects over a given range of years. This is illustrated in Figures 15–17 which are graphical representations of the number of references per annum during 1975 through 1984 (30 000 reactions) for the following general methods:

- (i) Asymmetric synthesis of the type



(Figure 15), which was searched with the keyword ASYM/PR

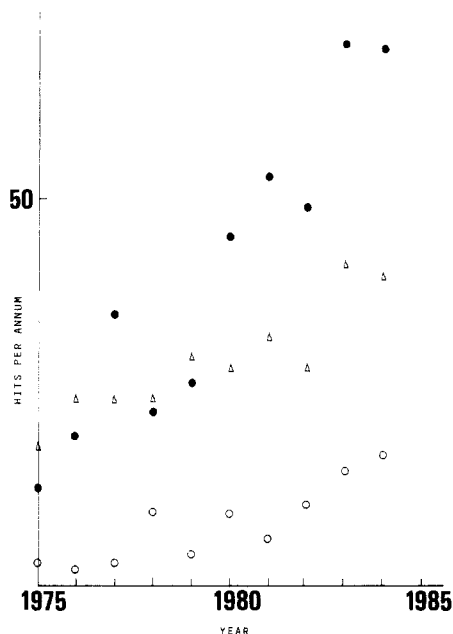


Figure 16. Graphical representation of a search for syntheses with organophosphorus (Δ), -silicon (\bullet), and -tin (\circ) compounds covering the period 1975–1984 (30 000 reactions).

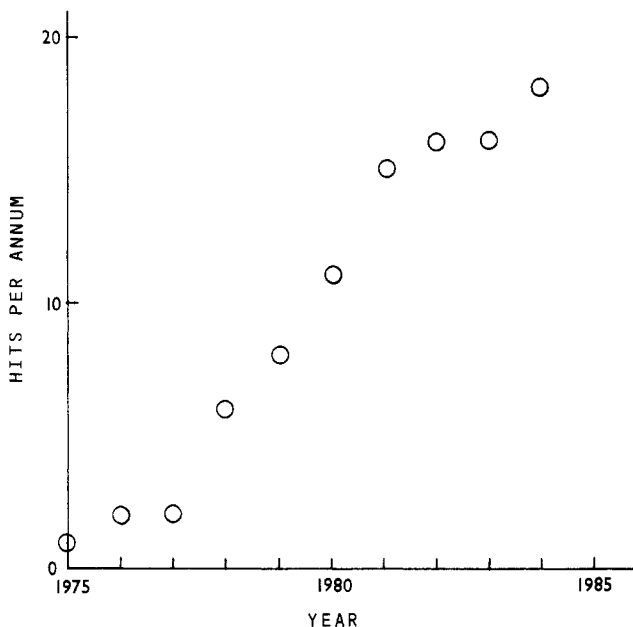


Figure 17. Graphical representation of a search for palladium-catalyzed syntheses with *O*-allyl derivatives covering the period 1975–1984 (30 000 reactions).

for all optically active products (C^*).

(ii) Syntheses of the type



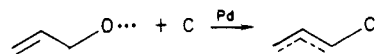
($Y = P, Si, \text{ or } Sn$; Figure 16), which was searched by combining a parameter for carbon-carbon bond formation (CC-X-M)⁶ with truncated keywords or terms for functional groups containing phosphorus, silicon, or tin as starting material:

(ALL PHOS:/SM OR P-YLID/SM) AND CC-X-M
for $Y = P$

ALL SI:/SM AND CC-X-M for $Y = Si$

TIN/SM AND CC-X-M for $Y = Sn$

(iii) Palladium-catalyzed syntheses with *O*-allyl derivatives of the type



for which the following search strategy was used:

ALLYL-O/SM AND

ALL ETHYLENE:/PR AND PD/RT

CONCLUSIONS

Services and systems providing data on synthetic methods should be comprehensive, up-to-date, inexpensive, and user-friendly. In our opinion, the CRDS—combining a database of more than 60 000 key reactions back to 1942 and the monthly JSM—fulfills the first two requirements. The cost to the user is a function of the annual subscription, online charges, and the technical time involved in designing search strategies and analyzing the data—none of which is great when one considers that it is often very difficult, and sometimes impossible, to obtain the same information by other means. User-friendliness cannot be assessed, though it would clearly be greater with a graphics system. In this respect, REACCS, the software developed by Molecular Design Limited,⁷ is particularly interesting and will shortly be marketed with a REACCS-compatible CRDS database for in-house retrieval. In addition, Derwent is considering the feasibility of mounting online a corresponding graphics-searchable reaction database, which may well see the light of day in the not-too-distant future. So too, no doubt, will other systems and services with varying claims and idiosyncrasies. Chemists will have the unenviable task of evaluating the merits of each, but those who do might recall that “...neither the easiest reaction documentation nor the most sophisticated is of any help to you if it does not include what you are looking for” (Theilheimer). Put another way, the ultimate factor is the quality of the database itself.

ACKNOWLEDGMENT

I am indebted to Dr. H. Birnbaum for helpful advice and guidance in preparing this paper.

REFERENCES AND NOTES

- (1) Theilheimer, W. “Synthetic Methods of Organic Chemistry”; Karger: Basel, Switzerland.
- (2) The *Journal of Synthetic Methods* is published by Derwent Publications Ltd., London, as part of the Chemical Reactions Documentation Service.
- (3) Reproduced from “Synthetic Methods of Organic Chemistry”, Vol. 38, with permission of Karger AG, Basel.
- (4) The Coding and Keywording are currently accessible via System Development Corp., 2500 Colorado Avenue, Santa Monica, CA 90406.
- (5) Schier, O.; et al. *Angew. Chem., Int. Ed. Engl.* **1970**, *9*, 599.
- (6) CC-X-M is the online notation for the reaction symbol CC↓↑Rem.
- (7) Molecular Design Limited, 2132 Farallon Drive, San Leandro, CA 94577.