

There is provision in the computer programs to delete or correct data when an occasional error in original recording may be found.

It is the ability of the computer to store, process, compare, search, and produce the completely interpreted record of the data that will make this system so useful to our Research Division.

## SUMMARY

Having our data on magnetic tape makes prescreening of compounds by computer possible. The computer can select those compounds which have desirable characteristics for testing in a specific screening program.

When a compound shows activity in some screening test we can easily pull from the tape file all similar compounds which have not been tested.

Complete records of compounds selected for screening may be printed out for review by an investigator. These records aid the investigator in planning his testing.

## LITERATURE CITED

- (1) Horowitz, P., Crane, E. M., "HECSAGON: A System for Computer Storage and Retrieval of Chemical Structure," Technical Memorandum, Kodak Research Laboratories, Rochester, N. Y., 1961.
- (2) Seitner, Philip G., Livingston, George A., Williams, Ann S., Eds., CBCC: Chemical-Biological Coordination Center Biology Code. A system for coding results, procedures, and conditions of tests for biological responses to chemicals, Publication 790 National Academy of Sciences, National Research Council, Washington 25, D. C. 1960.

# A New Information System for Organic Reactions\*

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**An information system for organic reactions on slotted punched cards for the use of the chemist in his laboratory is described. Using no new symbolism, it enables reactions to be found in the same simple manner as are chemical compounds, and provides information concerning structure and functions of initial and final products, reacting groups, reaction conditions, possibilities of synthesis, and side reactions.**

It is a truism to say that it has become impossible for an organic chemist to remember, assimilate, or even read every article which describes a new method of preparation in organic chemistry. That information—deriving from these sources—should be readily available, is nonetheless a pressing necessity. To acquire facts concerning organic reactions, we need a reference tool, from which it should be possible to ascertain directly the appropriate method to solve any particular problem of synthesis whenever the information is required.

What form should this information tool take?

A collection of information on chemical compounds presents no difficulties of principle. Each molecule is defined by its elementary composition and can therefore be traced either through its formula or its name. This latter method of identification may sometimes cause difficulty, but the problems involved are negligible compared with those encountered when the information required comprises

chemical reactions and methods of preparation, since a reaction cannot be defined as easily as a molecule. A chemical reaction is no static entity, but a transformation of one compound into another. Often, when a working method is being sought, it is not a question of merely reproducing the synthesis of another chemist, but rather one of finding the method which may be applied by analogy, with the greatest likelihood of success, to the synthesis of a new compound. Thus, the question is not one of recall, but of discovery.

If such data are sought by hunting for descriptions of synthesis of similar molecules—for example, by turning to the Formula Index of *Chemical Abstracts*—we run the risk of just missing the most promising methods, since, unfortunately, the analogous compound may be poorly selected; the publication which might have indicated the desired solution for a particular problem deals, for instance, with a compound which differs from the selected analogous compound only by the presence of a chlorine atom or a methyl group. Differences of this kind, which are small enough in themselves, constitute insuperable barriers to effective documentation, that are all the more dangerous because they are invisible.

\* Presented before the Division of Chemical Literature, 149th National Meeting of the American Chemical Society, Detroit, Mich., April 6, 1965.

\* As a result of the appreciated suggestion of Professor S. Hunig, the working methods borrowed from the periodical chemical literature will in future be quoted in unabridged form.

The textbooks and encyclopedias deal with organic reactions from different points of view—for example, by regrouping in a few great traditional classes reactions such as reduction, oxidation, degradation, and condensation. Such an abstract approach will very soon be blocked by the real complexity of reactions which sometimes are very individualistic.

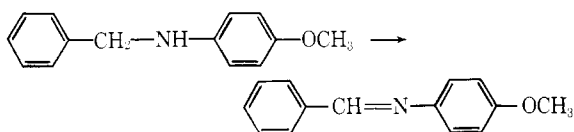
Now, from the point of view of functions obtained, this is an invaluable source of information. A problem arises, however, when several functions are to be introduced into the molecule. Which, then, are the functions to be introduced and which are the pre-existing functions in each stage of the synthesis? In other compilations the reactions are grouped according to their names or the names of their inventors.

Further types of reference works exist, but in any case, a disadvantage common to all of these textbooks and encyclopedias is that they are in the form of bound volumes which are quickly outdated by the advance of scientific progress; and the greater their bulk the sooner this is likely to happen.

#### PRINCIPLES: ASPECTS OF ORGANIC REACTIONS

If the problem of reference works relating to organic reactions is to be solved, the following double question should be asked at first: What are organic reactions, and what does the organic chemist wish to know about them from the point of view of preparation? This can be illustrated by a simple concrete example:

N-benzyl-4-methoxy aniline is dehydrogenated to the corresponding azomethine by means of  $\text{MnO}_2$  and azeotropic dehydration according to the method of E. F. Pratt and T. P. McGovern [*J. Org. Chem.* 29, 1540 (1964)]:



From the point of view of preparation, what may be stated concerning this reaction?

First, that two atoms of hydrogen are detached from the nitrogen and the neighboring carbon and a double bond is formed between these two atoms; the molecule is therefore partly transformed.

Second, that this transformation is produced by the action of  $\text{MnO}_2$  and the azeotropic elimination of the water formed.

Third, that the remainder of the molecule is left unchanged by the reaction.

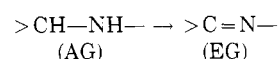
The  $\text{MnO}_2$  is a reaction partner for the same reason as is the organic amine, but, as it is an inorganic partner which does not contribute to the carbonaceous skeleton of the product of the reaction, it is considered to be an auxiliary reagent and is placed in the category of the "reaction conditions."

Generally speaking, this means the following: An organic reaction presents three preparation aspects:

1. The transformation of the reaction centers.
2. The reaction conditions.
3. The complete constitution of the reaction product.

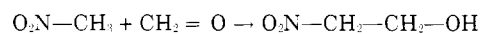
**Reaction Centers.** If reactions are considered to be a transformation of the reacting centers of the molecules which are made to react, every reaction may be designated by a pair of terms, the reaction center entering into reaction and the reaction center obtained; that is to say, the initial group (AG, Ausgangsgruppe) and the final group (EG, Endgruppe). The parts of the molecule which are not affected by the reaction are not taken into consideration.

In the above-mentioned example the "reaction-center equation" thus obtained appears as follows:

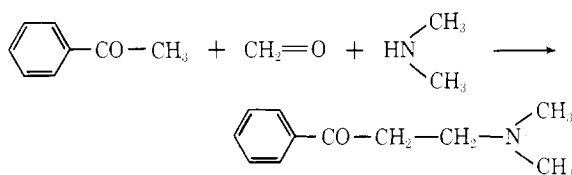


For constituting a means of reference in the matter of organic reactions, this way of looking at things offers several advantages:

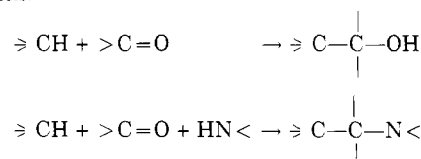
1. A reaction-center equation of this kind is a precise definition of concrete reaction type and dispenses with any systematization; there is no need to mention the type of reaction involved, whether it be one of substitution, addition, transposition, cleavage, or oxidation.
2. As the reaction-center equation disregards the nonreacting parts of the molecules, it often opens up the way of the formation of fruitful analogies. Thus the relationship between Henry's aldol addition



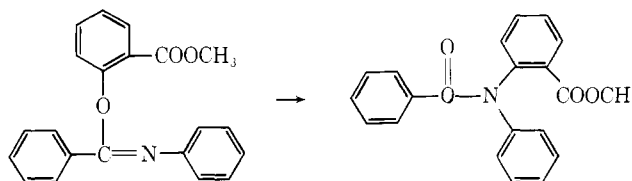
and Mannich's amino-ethylation



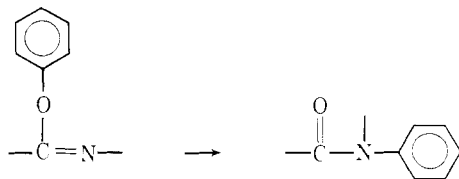
becomes obvious if these two complete reaction equations are changed into the corresponding Reaction-center equations:



3. As only the beginning and the end of a reaction and not the intervening pathway are considered, this conception remains independent of any hypothesis relating to the mechanism of reactions and is of permanent validity.
4. As the means of expression adopted is the one traditionally and habitually employed by chemists—namely formulas—no new symbols are resorted to.
5. Since reactions are indicated simply by means of chemical formulas, no problem concerning nomenclature or language is involved. Thus, the great trouble of trying to describe the Chapman rearrangement, for instance,

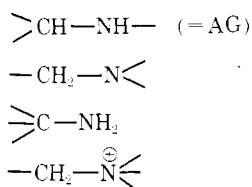


by a convenient and uniform nomenclature [J. W. Schulenberg, S. Archer, *Org. Reactions* 14, 3 (1965)] is irrelevant here, since it is defined by the following simple reaction-center equation:

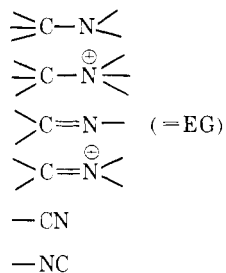


6. Although the initial reaction center (AG) and the final reaction center (EG) represent the dynamic character of the reactions, they are themselves static terms of concrete elementary composition and well defined as compounds. They may, therefore, be regrouped and traced according to either their functional or elementary composition. This means that any reaction may be traced in a register of chemical classification for compounds or even in a register of empirical formulas in exactly the same way as chemical compounds in the Formula Index of *Chemical Abstracts*. The only difference is that a product is defined by a single formula and a reaction by two or more. Thus, the aforementioned amine — azomethine dehydrogenation may be traced in the following sections of the empirical formula index of the reaction centers:

$\text{CH}_2\text{N}$ :



$\text{CN}$ :



7. This duplication of the reaction phenomenon in a pair consisting of the initial reaction center and the final reaction center enables countless organic reactions to be described by a limited number of formulas. It suffices to associate them according to the individual type of the reaction.

**Reaction Conditions.** The first aspect of organic reactions concerned their starting and finishing points. The second aspect concerns the path followed by the reaction between the initial and final stages. It is not related to the mechanism of this pathway, but to the practical, operational reaction conditions which define the pathway.

It has proved practical to group under the "chemical reaction conditions" concept both the reaction medium and the "auxiliary reagents," the latter term being understood to mean any reagent that does not supply carbon atoms to the product of the reaction. Thus, in the case

of chlorination in the presence of a catalytic quantity of dimethyl formamide, dimethyl formamide is included among the reaction conditions in the case of the Vilsmeier formylation (of thiophene ex. gr.), however, it enters as a reaction center into the reaction-center equation:



Furthermore, it was useful to make a separate note of "physical reaction conditions" such as irradiation, heating without a solvent, and the azeotropic elimination of the reaction water or of a volatile by-product. Thus, a photoreaction in the presence of benzophenone as a sensitizer can be recorded by the chemical reaction conditions "presence of benzophenone" and by the physical reaction conditions "UV irradiation" without using a particular code number for the fixed pair of notions "photoreaction + benzophenone."

**Reaction Products.** Although an organic reaction consists of a change of molecule, it is of interest for the organic chemist to know the parts of the molecules which have not changed.

Relevant information on reactions must therefore also comprise details about the complete constitution of the reaction products, not forming an over-all description including the empirical formula or an unsatisfactory nomenclature, but splitting up the subject into components which, in the view of the organic chemist, constitute reasonable and practical chemical entities.

The finished products are described by their skeleton and their functions.

Regarding the skeleton, there is not a great deal to be said. The degree of exactitude has been determined in accordance with the practical needs of the organic chemist.

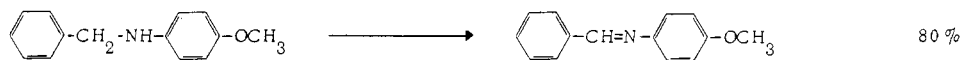
The functions are described by the following points: the valency of the function, the heteroatom by means of which the function is linked to the carbonaceous skeleton, and the character of the neighboring carbon atom.

Common functions such as the amine, hydroxy, carboxy groups, etc., are described in full.

#### PRACTICAL APPLICATION: "REACTIONES ORGANICAE"

If this way of considering organic reactions is translated into the concrete form of a punched card index, its simplicity and efficacy become still more apparent.

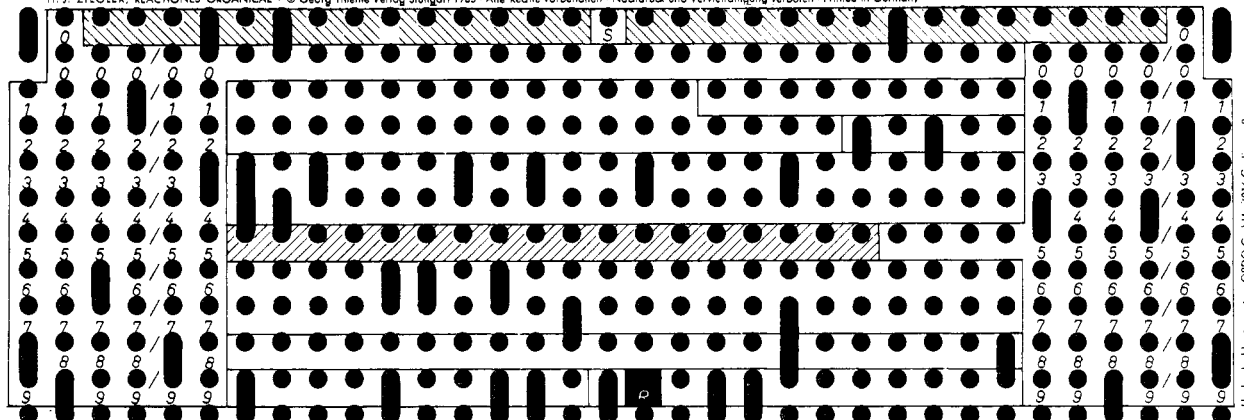
The following is a report concerning the slotted punched card index which I have elaborated according to the principles expounded and as a result of several years of experience and which has now been published under the name of "Reactiones Organicae" (by Georg Thieme Verlag, Stuttgart). Although this type of encyclopedia of reactions on punched cards exploits the most recent achievements in the field of card techniques, it does not require previous knowledge of computers and coding techniques, but treats the world of molecules and syntheses in the language and thinking of the organic chemist.



E. F. Pratt, T. P. Mc Govern

J. Org. Chem. 29, 1540 (1964)

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Benzal-4-methoxy-anilin

Kochen einer benzolischen Lösung von N-Benzyl-4-methoxy-anilin mit  $\text{MnO}_2$  (Herstellung beschrieben) unter azeotroper Entwässerung, Aufarbeitung.

A mixture of N-benzyl-p-anisidine,  $\text{MnO}_2$  and benzene heated while removing water by azeotropic distillation and worked up.

Ebenso:

Benzal-4-methyl-anilin	82 %	4-Nitro-benzalanilin	82 %
" -4-phenyl- "	91 %	4-Methoxy-	69 %
" -4-chlor- "	83 %	4-Methyl-	64 %
" - "	84 %	4-Chlor-	76 %
" -4-nitro- "	73 %		

u. a. m.

48

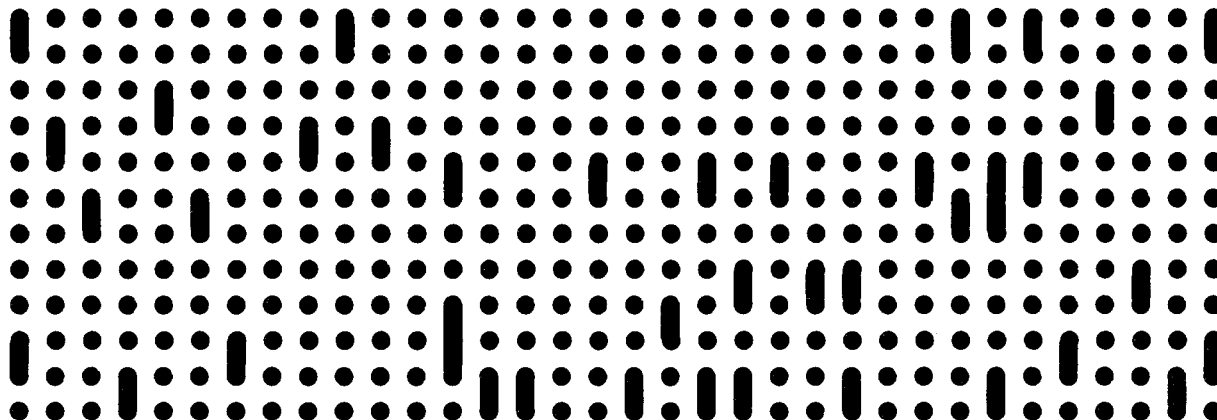


Figure 1. Front (top) and reverse (bottom) sides of card.

**General Description.** The "Reactiones Organicae" includes punched cards, a handbook with an introduction containing the necessary rules of the "game," two indices in the form of ring-books containing indices of initial groups and final groups (classed by chemical constitutions and by empirical formulas) and of reaction conditions, coding stencil-covers, a programming booklet, and a selector.

The cards employed are 14.5 by 21 cm. and made of IBM cardboard. Each card describes one reaction. The upper half of the card contains the plain-language text and the lower half comprises the punched area. The plain-language text provides the answers to the questions put via the punched area. This has 12 rows of holes with 34 holes in each row. A total of 374 holes can be used; there are no notches along the edges; the card is therefore strong and easy to manipulate.

The following data are clearly printed on the upper half of the card: In the middle part, the reaction is described by easily read graphic formulas and the yield and reference are given. To the left of the top border is the type of the reaction, expressed by the reaction-center equation; to the right are the reaction conditions and midway between the references to Houben-Weyl's "Methoden der organischen Chemie" (HW) and to the "Cahiers de Synthèse Organique" by J. Mathieu and A. Allais (CSO), and below these the name of the reaction (if there is one) taken from "Namenreaktionen der organischen Chemie" by H. Krauch and W. Kunz.

On the reverse side of the card are the name of the reaction product, the procedure\*, and other compounds which can be synthesized by the same procedure and their yields.

The first 3000 cards provide information about all the procedures in "Organic Syntheses," "Organic Reactions," "Cahiers de Synthèse Organique" and "Namenreaktionen der organischen Chemie." The cards will appear in the same order in which the reactions are dealt with in the Houben-Weyl volumes so that every group of cards covers a particular class of reactions.

Further cards (500 to 1000 every year) currently make available complete original texts on all the latest reactions

and procedures published in the international chemical literature only a short time after their appearance.

**Coding.** The coding of this data system is very simple. It corresponds to the various aspects of the reactions described above: the reaction centers, the reaction conditions, and the reaction products.

For greater facility in dealing with the 374 holes, the codes are not printed on the cards; they are indicated on stencil covers, each of which deals with a section of one of these reaction aspects: initial reaction centers (AG), final reaction centers (EG), reaction conditions (PC), molecule skeleton of the reaction products (M), etc.

They are applied to the punched area and only allow the part to appear whose code is printed on the appropriate stencil cover. To automate visually the selection of the stencil covers, they are differentiated by their color.

**REACTION CENTERS.** The reaction centers of the initial compounds and those of the finished products are recorded in the same way but independently of each other, the former by means of 96 holes and the latter by means of 109 holes. Two pieces of information are recorded in the case of each reaction center: (1) its individual formula and (2) the generic chemical class to which it belongs.

This is a tremendous advantage, as queries to the particular desired degree of detail can be posed. Thus in our example, the following questions can be asked of the card index:

How can I go from  $>\text{CH}-\text{NH}-$  to  $>\text{C}=\text{N}-$ , or even:

How can I go from amines to azomethines?

The most common reaction centers and their chemical classes are recorded by means of a single perforation, the others by means of six-figure code numbers; these are marked by six perforations in the same area of holes, even if several code numbers occur simultaneously. This "prime number check system" is a system of superimposed recording which is nevertheless free from risk of confusion and enables any reaction taking place between two or among several organic partners to be described easily.

In the present case, this system is comprised of the multiplication of the arithmetic series  $1, 2, 3, 4, \dots$  by 97, the last prime number below 100, and the use of the

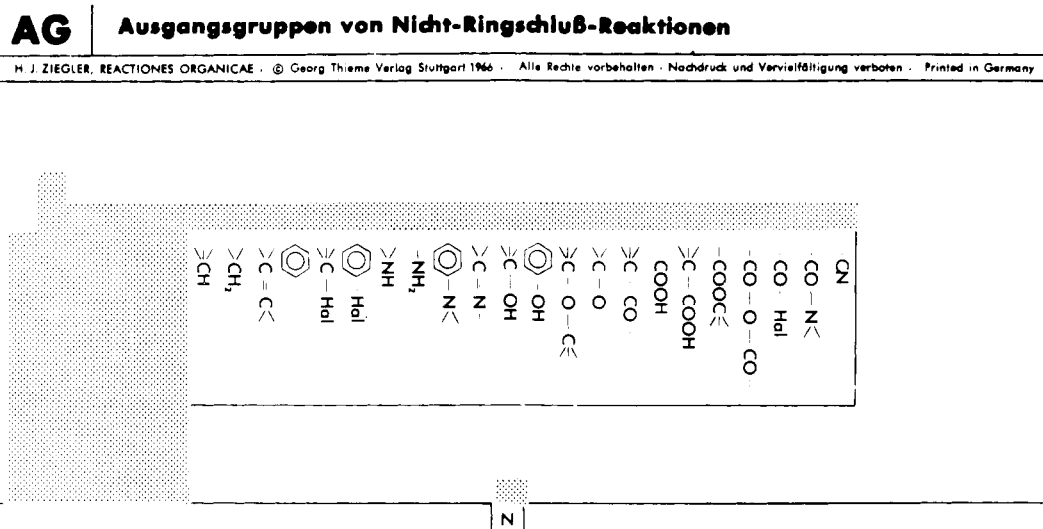


Figure 2. Coding stencil cover for initial reaction centers.

AG-Register	NO 29
8. Hydroxamsäuren	8186/80
$\begin{array}{c} \text{—C=N—} \\   \\ \text{NH—OH} \end{array}$	1903/14
9. Cyanate und Isocyanate	9293/25
$\begin{array}{c} \equiv \text{C—OCN} \\   \\ \text{—OCN} \end{array}$	2893/51
$\text{—NCO}$	3514/31
10. Urethane und Derivate	1818/75
$\begin{array}{c} \text{O} \\    \\ \text{N—C—OC}\equiv \end{array}$	4707/41
$\begin{array}{c} \text{O} \\    \\ \text{—NH—C—OC}\equiv \end{array}$	5138/09
$\begin{array}{c} \text{O} \\   \\ \text{NH}_2\text{—C—OC}\equiv \end{array}$	6969/45
$\begin{array}{c} \text{O} \\    \\ \text{C}=\text{C—N—C—OC}\equiv \end{array}$	7622/26
$\begin{array}{c} \text{O} \\    \\ \text{C}=\text{N—C—OC}\equiv \\   \\ \text{N—C—OC}\equiv \\   \\ \text{O} \end{array}$	8794/02
$\begin{array}{c} \text{COOC}\equiv \\   \\ \text{N—C—OC}\equiv \\   \\ \text{COOC}\equiv \end{array}$	9131/58
$\begin{array}{c} \text{O} \\    \\ \text{CO—C—NH—NH—C—OC}\equiv \\    \\ \text{O} \end{array}$	1089/31
11. N-Nitroverbindungen	2394/93
$\text{N—NO}$	2502/60
$\begin{array}{c} \text{NO} \\   \\ \text{CH—C—N—CH}\equiv \end{array}$	3334/86
$\text{—N—NO}$	4278/67
$\begin{array}{c} \text{ON} \quad \text{O} \\    \quad    \\ \text{CH—N—C—} \end{array}$	5943/19

Figure 3. Sample page of the index of initial reaction centers' classed chemically (AG).

EG-Register

O 42

11. Carbonylgruppen

11.1. Eine Carbonylgruppe

Direkt-Zuordnung

11.1.1. Isolierte Carbonylgruppe

$\text{>C=O}$

Direkt-Zuordnung

$\text{-CH=O}$

Direkt-Zuordnung

$\equiv\text{C}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

Direkt-Zuordnung

$\text{>CH}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

Direkt-Zuordnung

$\text{-CH}_2-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

1256/15

$\equiv\text{C}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

9196/37

$\text{>C}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

0161/02

$\text{>CH}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

1180/49

$\text{>CH}-\overset{\overset{\text{O}}{\parallel}}{\text{CH}}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

2931/34

$\text{>CH}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-\overset{\overset{\text{O}}{\parallel}}{\text{CH}}=\text{O}$

3463/87

$\equiv\text{C}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\text{C}\equiv\text{C}$

4561/91

$\equiv\text{C}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\text{CH}\equiv\text{C}$

$\equiv\text{C}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

5954/83

$\text{>C}=\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-$

1229/96

$\text{-}\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\underset{|}{\text{C}}}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}=\text{N}-$

Siehe N/3.

Figure 4. Sample page of the index of final reaction centers classed chemically (EG).

Chemische Reaktionsbedingungen		3...
<b>6. Elemente</b>		
(einschließlich $H_2$ , ausschließlich der Alkali- und Erdalkalielemente und Al)		
Wenn nicht anders vermerkt, stehen die Legierungen unter dem Metall mit der niedrigsten Ordnungszahl; die Amalgame stehen unter Hg.		
<b>H:</b>		50
Hydrierapparat, Benutzung und Eichung: O. S. I, 61		
$H_2 + LiP_2O_4$		5000
" $+ Cu_2P_2O_4$ oder $BaCr_2O_4$		5001
" $+ Raney-Ni$ (O. S. III, 181; O. S. <u>21</u> , 15) oder andere Ni-Katalysatoren		5002
" $+ Raney-Ni + NH_3$		5003
" $+ Ni-Cu$		5004
" $+ Co$ -Carbonyl		5005
" $+ Raney-Co$ oder andere Co-Katalysatoren		5006
" $+ Rh-Al_2O_3$		5007
" $+ Pd (PdO)$ (PdO: O. S. II, 566)		5008
" $+ Pd$ -Kohle (Pd-Kohle: O. S. III, 685; <u>26</u> , 77) (evtl. + andere Hilfsstoffe, z. B. HOAc + Spur konz. $H_2SO_4$ )		5009
" $+ Pd-BaSO_4$ (Pd-BaSO <sub>4</sub> : O. S. III, 685; <u>28</u> , 77) (evtl. + Chinolin-S)		5010
" $+ Pd + Piperidin$		5011
" $+ Pd + HOAc + Pyridin$		5012
" $+ Pt (PtO_2)$ (PtO <sub>2</sub> · H <sub>2</sub> O: O. S. I, 463; 466, Note 9; Rückgewinnung: Inorg. Synth. <u>7</u> , 232)		5013
" $+ Pt^{II} + NaBH_4$		5014
<b>O:</b>		
$O_2$		51...
$O_2$ oder Luftsauerstoff allein		5100
" $+ Säuren$		5101
" $+ Alkalien$ (evtl. + Metalloxyde)		5102
" $+ V_2O_5$ oder andere Metalloxyde		5103
" $+ CuCl, NH_4Cl + wässr. HCl$		5104
" $+ NH_4OH$ (evtl. + Cu)		5105
" $+ NH_3 + Pt$		5106
" $+ Pb (OAc)_4$	Siehe 8. /Pt	
" $+ Dimethylsulfoxyd$		5107
$O_3$		520...
$O_3$ allein (O. S. III, 673; <u>26</u> , 63)		5200
" $+ HCl$		5201
" $+ HCOOH$		5202
" $+ Jod + IOAc$		5203
		5204

Figure 5. Sample page of reaction condition index (PC).

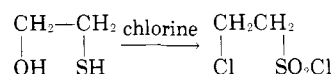
product numbers thus obtained as code numbers. The first 10,000 product numbers are employed for the 10,000 reaction centers provided for in this data system. As a result of the multiplication by 97, each product number contains two extra figures which do not have the signification of a code number but which permit recording by means of superposition while avoiding the coincidence of simultaneous recordings. We may compare these two auxiliary figures with the wave frequency by means of which several telegraphic signals may be simultaneously transmitted along the same wire.

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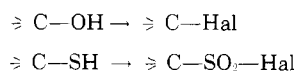
1 x 97 =    97 ..... 0000/97
2 x 97 =   194 ..... 0001/94
3 x 97 =   291 ..... 0002/91
4 x 97 =   388 ..... 0003/88
.
.
.
.
10309 x 97 = 99973 ..... 9999/73
prime number check system

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The prime number system also enables reactions with several reaction centers in the same molecule to be recorded—for instance



Both of these reaction-center equations defining this reaction



can be noted directly and simultaneously on one and the same card and thus also be traced in combination.

This arrangement provides very valuable information from the point of view of preparation.

Of the  $2 \times 10,000$  possible recordings (10,000 for the initial reaction centers and 10,000 for the final reactions centers), only about 8% are at present utilized; the remaining 92% constitute a future reserve.

The code numbers are traced either in the registers of the reaction centers, classed chemically, or in the collective register for the initial and final reaction centers, classed according to empirical formulas. Any type of reaction whatsoever may be sought by combining initial reaction centers with the final reaction centers.

However, in the case of cyclizing reactions this code would lead up a blind alley, as the formula of the reaction centers would then lose their simplicity and visual clarity. Ring formations are therefore described by indicating the significant elements of the cyclizing molecules on the one hand and of the rings obtained on the other. The idea is the same as for the noncyclizing reactions, the subdivision of the reaction into two terms: the starting point and the finishing point.

To employ the same holes for the cyclizing reactions as for the noncyclizing reactions, it is only necessary to perforate the holes R and N (in the lowest row of holes), respectively.

**REACTION CONDITIONS.** Each reaction is defined by a single group of physical and chemical reaction conditions. Recording by means of decimal code (S1247 System) is therefore sufficient: 10 possibilities have been foreseen for

the physical conditions and 10,000 for the chemical conditions. Until now, about 11% of the total recording capacity has been utilized. The classification of the chemical conditions enables the selection to be accomplished not only according to individual and very precise conditions—for instance,  $\text{NaBH}_4$ —but also according to more general groups such as the hydrides or the bases in general.

**REACTION PRODUCTS.** The characteristic features of the molecular skeleton (M) and the functions (F) of the reaction products are recorded by direct code indicated on the coding stencil cover M and F.

**PERSONAL NOTATIONS.** The card-index user may record his personal notations, whether chemical, administrative, or others, in 18 holes either by direct code or by decimal and alphabetical codes, according to individual requirements. To deal with quite special reactions, perforate hole S (in the middle of the top row of holes), thus reserving 205 holes for reaction centers in a particular field.

**Selection Operation.** Selection is effected by means of a programming booklet. By way of illustration, the originally mentioned example of amine dehydrogenation to azomethine may be chosen. It is written at the top of the programming booklet.

Next, one looks up the corresponding code numbers in the indices, then one formulates the problem in the language of these code numbers in the second space of the programming booklet sheet and, finally, with a colored pencil, one crosses out the corresponding holes in the punched area section of the programming booklet. One tears off this punched area section, places it on the front plate of the selector, inserts needles into the crossed holes and subjects packs of 250 to 500 cards to the selection operation.

One thousand cards are easily sorted within three minutes; and when this mechanical selection has been made, the user has the clear texts before him—that is to say, his notes have been made and he does not even have to translate code numbers or search for cards in a master card index.

<b>M Molekülskelett</b>	
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<b>Aliphat.</b> <div style="display: flex; justify-content: space-around;"> <div> </div> <div>           Nur aliphat.            An Alicycl.            An heterocycl. C         </div> </div>	<b>Ringanordnung</b> <div style="display: flex; justify-content: space-around;"> <div>           ortho- peri- Ster. u. Sop.  </div> <div>           Brücken            Kondensierter Ring            Überlappende            Valenzbrücke            Atombrücke            Andere         </div> </div>
<div style="display: flex; justify-content: space-around;"> <div>           = 1/2 -  <b>Carbo-</b>  <b>cyclen</b> </div> <div>           = 1/2 -  <b>Bdg.-Syst.</b> </div> <div>           N O S And. At. gr. 1 &gt; 1  <b>Atomarten pro Ring</b> </div> </div>	<div style="display: flex; justify-content: space-around;"> <div>           1 2 &gt; 2  <b>Heteroat./R</b> </div> <div>           BK 1,2 1,3 1,4  <b>Stellung</b> </div> </div>
<b>Heterocyclen</b>	
<b>Ringzahl in kondens. Ringsystemen</b> 2 3 4 5 > 5 Insgesamt	<b>Ringgröße</b> 2 3 > 3 0 1 2 > 2 Gleich gr. R. Heterocyclen
<b>Atome zwischen Ringsystemen</b> 0 1 2	

Figure 6. Coding stencil cover M for the molecule skeleton of the reaction product.

**S****Eintragungen des Karteibenzutzers**

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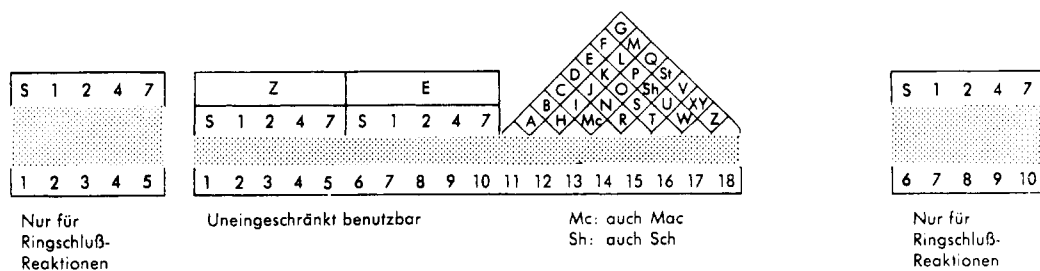


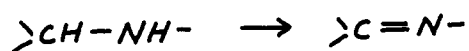
Figure 7. Coding stencil cover S for special personal notations.

**Programmierblock**

Programing booklet

Problemstellung:

Query

No. **58***Amine → Azomethine Dehydrogenation*Codierung:  
CodingNo. **58**

$$8961/83 \rightarrow 4194/28$$

AC                      EC

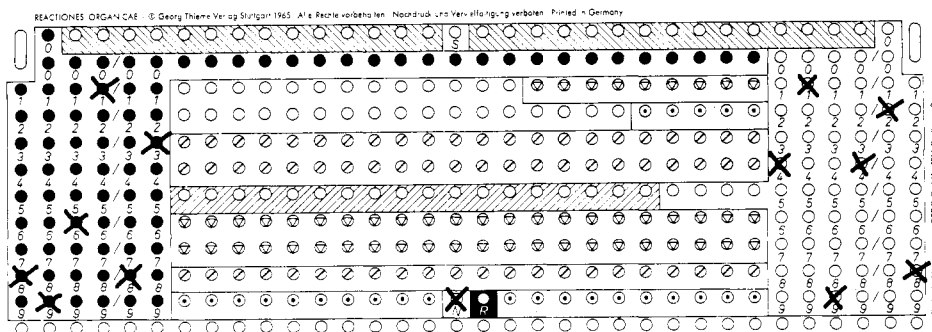
Nadelung:  
Needle SortingNo. **58**

Figure 8. Programming booklet.



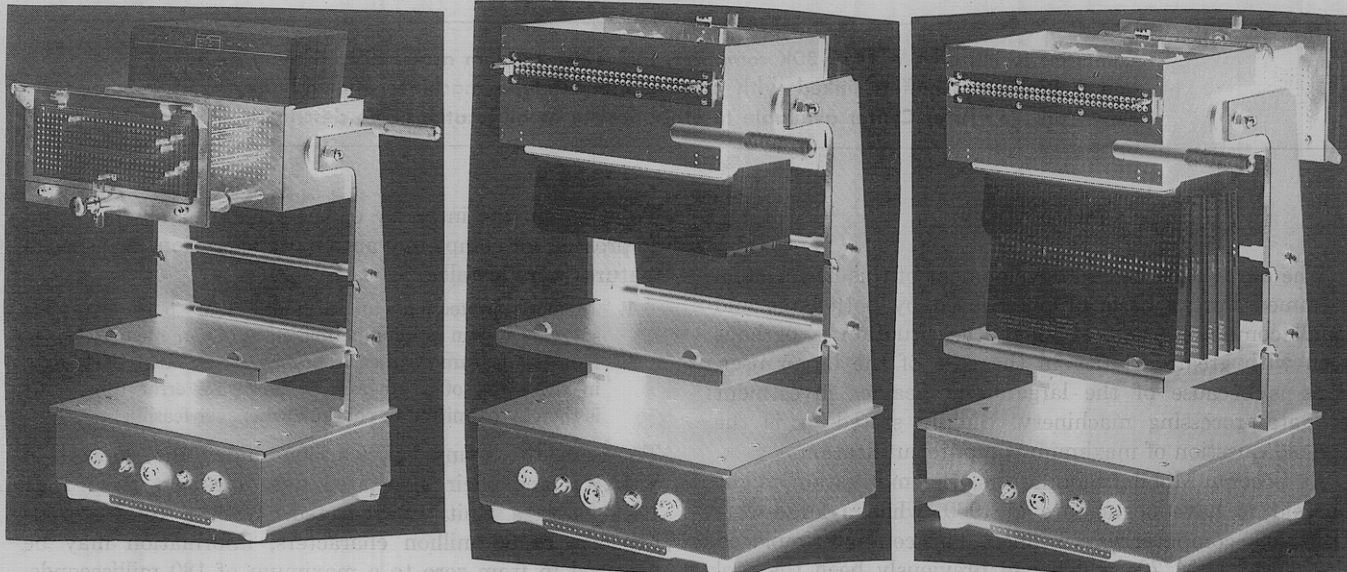


Figure 9. Operation of the selector from programming sheet

First stage: A programming sheet placed on the selector and needled; a pack of cards inserted in the selector.

Second stage: The selected cards protruding downwards.

Third stage: The selected cards completely separated.

### APPLICATIONS

This information system answers varied questions relating to a single notion or any possible combination of notions according to the needs of the moment. Here are a few questions to illustrate the capacities of this tool:

How can I condense a carbonyl group with a methylene group to form an olefin double bond?

Which methods can be used to convert a carbonyl compound into an olefin?

By which methods can olefin double bonds be produced?

How can acetophenones be halogenated in the ring, and how in the  $\omega$ -position?

How can C-alkylation be effected without simultaneous alkylation of hydroxy group?

Which reaction can be effected with metal hydrides?

How can I prepare *tert*-butyl chloride?

How can the ester group of peptides be saponified without hydrolyzing the peptide bridge?

### ACKNOWLEDGMENT

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## SMART (Socony Mobil Automatic Real Time) Computer System\*

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Until only recently, the phrase "real time" among computer users had come to be associated with highly specialized government applications, for example, in the guided missile and space satellite projects. The extremely large investment in computer hardware, system software, and communication facilities for such projects precluded the application of this concept to commercial areas for many years.

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At Socony Mobil Oil Company headquarters, however, this advanced concept has been turned inward, as it were. Late in 1962, the SMART computer-communications system was put into operation which enabled Socony personnel at remote locations to transmit data to the computer center, direct the computer to perform certain computational and/or retrieval functions, and to receive "answers" in a matter of seconds. The objective was to improve computer utilization by significantly reducing the "turn-around time" previously existing between the moment when an "order" for services was received at the computer center and the time when it was fulfilled.