particle. None of the other particles which appear and disappear during the previous development stages of the shower can be measured by this apparatus. But since the shower particles possess enormous energies, they are capable of producing radiation in the air of the type under discussion, which is propagated in virtually the same direction. This radiation, under favorable conditions, reaches the earth's surface and can be measured by a photomultiplier. This method furnishes a more complete picture of the shower and valuable information about the process of its development.

For cosmology, the problem of the distribution of nuclei in the cosmic radiation (outside the earth's atmosphere) which are heavier than the hydrogen nucleus is of great importance. Appropriate experiments are being carried out on the sputniks at the present time. In these experiments, reliance is placed on the circumstance that the intensity of the radiation of particles which move with superlight velocity is proportional to the square of the particle's charge. Therefore, the pulses coming from particles of different charges and recorded by the counter may be distinguished by their amplitudes. Analysis of the amplitude distribution will permit one to make judgments on the distribution of heavy particles in the cosmic radiation, corresponding to their ordinal number.

The last thing on which I would like to speak is the application of the radiation from fast-moving particles to measurement of the energy itself when this energy is rather large. In this case measurement of the energy of the particles by means of their deflection in a magnetic field is no longer possible. However, one can try to determine it by measuring the total energy which the particle gives to the radiation of the type under consideration. For this purpose, very transparent, thick radiators must be used, which give off radiation of a sufficient intensity and which permit a complete development of the shower.

Water is a suitable radiator in this case. Equipment has been constructed in the Institute of Physics, Academy of Sciences of the U.S.S.R., which should serve for the measurement of the energy of cosmic particles by means of this method.

The examples we have given show the great importance to experimental physics of the radiation produced by particles which travel with superlight velocity (*17*).

However, not all the possible applications have been discussed. It is undoubtedly true that the region of application of this radiation will continue to expand rapidly in the years to come.

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Machine Searching for Chemical Structures

The Wiswesser notation provides an effective key to literature searches for functional groups.

Elbert G. Smith

The use of punched-card machines for organizing and retrieving chemical data has been described by a number of workers in recent years (*1*). These techniques make it possible to find and arrange information about large numbers of items very rapidly and efficiently, provided that the information about each item is not too extensive. Since this is precisely the situation we face in dealing with data about chemical compounds (large numbers of compounds but rather limited data, such as structure or properties, about each one), it would seem feasible to organize and search this kind of information with punched-card techniques.

A principal difficulty has been that of devising a means of identifying chemical compounds in an intelligible way which is concise enough for efficient use on punched cards. Ordinary names are usually too long to be efficient and do not allow use of the machine's potential ability to search for units of molecular structure in the identifying name. A solution of this difficulty lies in the concept of a new chemical notation in which units of chemical structure are designated by single letters and numbers, so that structural formulas may be spelled out much as one spells out words. Such notations can be designed so that they are intelligible both to the chemist and to the machine, and in such a happy combination we might look for practical and reasonable means of accomplishing the mechanical organization and retrieval of much chemical information.

The author, now associate professor of chemistry at Mills College, Oakland, Calif., did the work described in this article at the University of Hawaii, Honolulu.

Wiswesser Notation

The Wiswesser notation (*2*) meets these requirements very well. It is intelligible at sight to any chemist who will learn about a dozen new symbols to supplement the old familiar ones and some of the more essential rules for using them. It is also intelligible to punched-card machines because it does not use any symbols that cannot be expressed on existing machines. It is so concise that at least 98 percent of the organic compounds of known structure in such a compilation as *Heilbron* can be expressed in notations which require less than half of the information space on a single IBM card. The rest of the card then can carry other information about the compound, and the resulting single card for a single compound greatly simplifies the machine problems in finding and reproducing desired information. No other notation yet proposed can meet so well these essential requirements of intelligibility and conciseness.

The Wiswesser notation gives unique patterns of letters and numbers for each different structural formula, so there is only one place to look in any alphabetically arranged list of notations for any given compound. The problem of locating data about a specific compound is thus solved directly by the notation itself. Searching for groups of compounds with the same functional groups is more difficult, however, since symbols for a particular functional group may occur at any point in the line-formula notation and so may occupy any column or group of columns in the part of an IBM card punched with the notation. Since punched-card machines do not scan the card lengthwise along the notation but at right angles to it along one or more vertical card columns (each representing a single letter or number), all the cards would have to be sorted in all the columns of the notation field (and letters require double sorting) to find all the cards carrying a particular notation symbol. This would be such a tedious and time-consuming operation that machine searching of cards for groups of compounds with similar functional groups would be an impossible undertaking. To make matters worse, only very expensive types of machines can scan more than one card column (and so find more than one notation symbol) at a time. If the desirable properties of the Wiswesser notation are to be used to advantage, they therefore must be supplemented by some additional searching code adapted to finding the cards carrying particular symbols, preferably by use of the simpler and less expensive, single-column sorting machines.

Table 1. Two column code for showing elementary atom count.

Punch position	Column 1 No. of carbon atoms	Column 2 No. of other-element atoms
12	10	1 Oxygen
11	20	2 Oxygen
0	40	4 Oxygen
1	1	8 Oxygen
2	2	1 Nitrogen
3	3	2 Nitrogen
4	4	4 Nitrogen
5	5	1 Halogen
6	6	2 Halogen
7	7	4 Halogen
8	8	1 Other
9	9	2 Other

Searching Code Proposals

Wiswesser (*4*) has suggested a code of this kind in which each letter symbol from the notation for a particular compound is indicated by a single punch in one of 26 fixed positions in a three-column section of the punched card. Thus, cards with notations containing the symbol V (the carbonyl connective, –CO•–) would be punched in position 5 of column 3, and cards containing the symbol M (the –NH– group) would be punched in position 4 of column 2. By a single sort of the card file for position 5 in column 3, all cards for compounds containing carbonyl connective groups could be removed. If one desired to find compounds with the structure –CO•NH– (-VM- in Wiswesser notation), the cards found on the first sort (for V) would then be searched for M symbols by sorting them on position 4 in column 2.

Unfortunately, in practice, entirely too many unwanted cards are produced by such a searching code, particularly if one is searching for single-symbol functional groups. A search for ketones (V) would also produce many cards for compounds carrying V symbols in other functional groups which are not ketones at all—amides, ureides, anhydrides, acid halides, and so on. In other words, the simple letter code is not sufficiently selective to do a satisfactory job. At the same time, some of the positions in this searching field proposed by Wiswesser are either very seldom used or are meaningless in terms of organic molecular structures (*5*).

For these reasons a modification of this searching code was devised on the basis of exhaustive frequency counts of symbols and symbol combinations in the Wiswesser notations for some 10,000 common organic compounds. This code has been tested and revised a number of times during the past six years on a continually growing punched-card catalog of organic notations which now contains data on 50,000 compounds. A number of machine searches were carried out when the catalog contained 24,700 compounds, and another series was run when the catalog had been expanded to 50,000 compounds. The resulting searching code, presented in Tables 1 and 2, is thus a strictly practical effort to facilitate the finding of compounds with particular structures. Each definition in Table 2 is the result of some years of experience with the problems involved.

The searching code so evolved was punched into the first five columns of the IBM cards used, and so the columns in Tables 1 and 2 are numbered accordingly. Table 1 shows the code used to record the carbon, oxygen, nitrogen, halogen, and "other atom" counts. With multiple punching in the top three positions in column 1, up to 79 carbon atoms can be indicated. Multiple punching within each group in column 2 will indicate up to 15 oxygen atoms, 7 nitrogen atoms, 7 halogen atoms, and 3 other atoms. In each case the maximum number is used to indicate that number or more of the atom in question. No difficulties have been found in practice for the rather minor use made of this part of the searching code.

Structure-Searching Code

The real heart of the searching method is the three-column structure-searching code shown in Table 2. Each column has 12 punching positions, and the categories are arranged according to elementary type. One of the 36 positions is unassigned so that it may be used for special purposes where needed. As shown in Table 2, the 35 categories fall into two classes: (i) symbols or groups of symbols which commonly occur alone in organic notations of a given functional type (acids, ketones, ethers, esters, and so on) and (ii) symbols or groups of symbols which can be combined with each other to express more complex functional groups (sulfonic acids, ox-

imes, amides, anhydrides, and so on).

For example, the symbol Q, denoting the –OH group, occurs alone in phenols (column 4, punch position 4) and in alcohols and enols (column 4, punch position 5). The Q symbol also occurs in combination with other symbols in oximes, sulfonic acids, some inorganic acids, the carboxyl group, and so on. Unless separate searching-code positions are assigned to Q symbols in phenols and alcohols, these cards cannot be separated effectively from each other or from cards for oximes, sulfonic acids, and so on. By assigning a separate punch to "Q attached to non-carbon atoms" (column 4, punch position 6), this difficulty is solved and at the same time the number of Q cards that must be dealt with in a given search is greatly reduced.

Searching Procedures

In the first class of categories mentioned above it is clear that highly efficient searches for compounds with more than one functional group can be carried out. For example, if one wants the cards for unsaturated acids containing bromine atoms, the card file would be run through the sorting machine with the sorting switches set to select only the cards punched in column 3, punch position 0 for E (bromine). The cards so selected would then be sorted on column 5, punch position 12 for U (unsaturation). The cards selected on this sort would then be sorted on column 4, punch position 12 for QV (acids). This would produce all the cards in the entire file which carry notations with the three structural units desired. Obviously, in this type of search, no unwanted cards could be produced. In other words, the searching efficiency would be 100 percent with the machine alone.

In the second class of categories the searching efficiency is usually less, but the searching procedures are more interesting since they require a bit more ingenuity. For example, in searching the "Q attached to non-carbon" category for various functional groups containing the Q symbol, separations are made by sorting for the other symbols combining with Q in the functional group desired. In searching for sulfonic acids (WSQ- or -SWQ in Wiswesser notation), the Q cards are sorted for WS symbols (column 5, punch position 2). Only those cards so selected can carry sulfonic acid notations. In searching for oximes (QNU- or -UNQ in Wiswesser notation), the cards carrying Q symbols are sorted for "N attached to one or two non-keto carbons" (column 3, punch position 7), and the cards so selected are sorted finally for "U attached to non-carbon" (column 5, punch position 11). Only the cards so selected can carry notations of oximes.

Unwanted Cards

In three-step searches of this kind there is an astonishingly small number of unwanted cards—those carrying random coincidences of the desired symbols in undesired combinations. In searching for oximes among 24,700 compounds of all types, 629 cards were found by the three-step sorting procedure described above. Inspection of the notations showed that 612 were oximes. The unwanted cards often can be removed mechanically by sorting for unwanted symbols that commonly occur attached to one of the wanted symbols. In this case the 629 cards were sorted for WS symbols (column 5, punch position 2), since these commonly occur with Q symbols in sulfonic acids. This sort produced 13 cards; one of these was an oxime but the other 12 were not. Thus the "contamination" was reduced to five unwanted cards, among cards for the 612 oximes actually present, by a purely mechanical operation.

In general, the more symbols one can specify for a given search, the fewer unwanted cards one obtains. In a search for semicarbazones, $H_2N{\cdot}CO{\cdot}NH{\cdot}N$: (ZVMNU- or -UNMVZ in Wiswesser notation), where four searching-code categories are specified—Z, MV, N, and U—350 cards were found in the four-step sorting of the 24,700-compound file. All but one of the 350 were semicarbazones. This is not a selected example; this is exactly the probable contamination one might predict statisically from the frequency counts of the four categories shown in Table 2. As verification, a similar search for semicarbazones was made when the catalog had reached 50,000 compounds. The four-step sorting produced 1097 cards, and all but two were semicarbazones.

Searching Time

The total time required for a search depends partly on the speed of the sorting machine, partly on the sorting sequence chosen, and partly on the amount of visual inspection of the notations that is needed. Searches obviously should start on the symbol with the lowest frequency in Table 2, so that the greatest possible number of unwanted cards will be removed on the first pass through the sorter. The most commonly used IBM sorter, with a speed of 650 cards per minute, required from 35 to 40 minutes to sort the deck of 24,700 cards. In a later phase of this work a sorter with a 1000-card-per-minute speed became available, and this required just under an hour to sort the 50,000 card deck.

Category Decks

Since this first step in a search is obviously the most time-consuming, a means of eliminating it was sought. The total number of searching-code punches, calculated from the frequency counts in Table 2, is only about 2.9 times the total number of compounds. If one omits the least discriminating (U-non-carbon and Y) categories, this factor is reduced to about 2.5 punches per compound. The same factor of 2.5 was found at both the 24,700- and the 50,000-compound levels. This relatively small factor suggested a simple way to avoid repeated sorting of the entire catalog: sort out each category in turn, duplicate the cards, and keep each of these new category decks in a separate card file. In this way the entire deck never need be sorted again, and each category deck is available at once for any searches in which it is needed. As new compounds are added to the file, the additional cards for each category deck file are easily prepared and filed in their appropriate decks. This duplication by categories not only saves much time in searching but avoids wear and tear on the master cards. These can be kept in alphabetical order by notation for rapid location of individual compounds, for assigning card serial numbers to new entries, and for other purposes. Card duplication of this sort is purely mechanical with an appropriate IBM machine and is foolproof and inexpensive. The relatively low card multiplication factor of 2.5 makes this a feasible and economical procedure.

Some Functional Group Searches

Many searches can be speeded further by keeping the cards in alphabetical order within each category deck. In the search for oximes among 24,700 com-

pounds, the Q-non-carbon category deck of 1451 cards was used. About 300 of these carried notations beginning with the desired combination, QNU-. Removal of these from the category deck left less than 1200 to be sorted for the N and U category symbols on the sorting machine. The first sort on the machine required about 2 minutes, and the entire search was completed in less than 5 minutes.

In the semicarbazone search on 24,700 compounds described above, the MV-non-carbon category deck of 827 cards was used. The cards with notations starting with ZVMNU- were quickly removed by visual inspection of the alphabetized deck, and the remaining cards were sorted for the Z, N, and U punches. The cards so selected were alphabetized by sorting on a serial number punched in the cards for this purpose. These cards were added to those in the ZVMNU- group, which were already in alphabetical order, and the entire group was run through an IBM tabulating machine which listed all of the printable data from the cards. The entire operation, starting with the alphabetized MV category deck and finishing with an alphabetized, printed list of semicarbazones, required only 15 minutes. The cards for semicarbazones were then arranged mechanically by melting point of the compound, in ascending order, and listed on the tabulating machine in this order. This required another 15 minutes. With a more modern tabulator than was available for this work, and with continuous-feed printing forms, the listing time could have been materially reduced.

Control of Unwanted Cards

Searches involving only two symbol specifications produce a larger number of unwanted cards, but alphabetized category decks permit visual removal of wanted and unwanted portions, and this accelerates the mechanical search. For example, in searching 24,700 compounds for unsubstituted amides, $-CO{\cdot}NH_2$ (-VZ or ZV- in Wiswesser notation), the V-non-carbon category deck of 1536 cards was used, since this was smaller than the Z deck. Removal of the desired cards with notations beginning with ZV- left some 1200 cards to be searched mechanically for Z in column 3, punch position 9. This sort produced only 100 cards carrying both Z and V symbols in which visual inspection for -VZ combinations was necessary. Visual inspection of the ZV- group allowed quick removal of some unwanted ZVM-, ZVN-, and ZVS- combinations. The search was completed in 7 or 8 minutes.

Selection of symbols nearer the beginning of the alphabet is a bit more difficult because the basic orienting rule of the Wiswesser notation tends to place these in terminating rather than in initiating (and therefore alphabetically obvious) positions in the line-formula notation. A search for acyl chlorides illustrates this, as some 42 percent of the acyl chloride notations show -VG at the ending, rather than GV- at the beginning, of the notations. This search started with the 1536 cards in the alphabetized V-non-carbon category deck. These were inspected visually for notations beginning with GV-, and 116 cards were found and removed. The remaining cards were then searched mechanically for G by sorting for punch position 11 in column 3. About 250 cards were found. These were inspected visually for -VG groups, and 84 of the desired cards were found. This inspection required about 5 minutes. While the sorter was searching for G among the V cards, the initial GV- cards were inspected, and one beginning with GVN- (not an acyl halide) was found and removed. In this way 199 acyl halides were located in less than 10 minutes, despite the unfavorable circumstances of a two-symbol combination with nearly half not in initial positions in the notation.

The 199 acyl halide cards, still in alphabetical order by notation, were run through the tabulator for listing in this order. Then the cards were arranged mechanically by boiling point of the compound, in ascending order, and listed in this order. Next the cards were

Table 2. IBM code for searching chemical structure descriptions in Wiswesser notation. Capital letters are Wiswesser symbols. A hyphen after the symbol means "attached to" the atom or group shown. Figures in parentheses show the observed frequency of each category in 50,000 organic compounds.

Punch position	Presence of group is shown by punched position in		
	Column 3	Column 4	Column 5
12	G (chlorine atom), ionic or inorganic (2945)	QV (—COOH acids) (6940)	U (unsaturation)-carbon only; CC if equivalent to UU (5164)
11	G, all other chlorine (5548)	OV-two non-keto carbons (esters) (9204)	U-non-carbon (7014)
0	E (bromine atom) (4299)	OV-non-carbon or ionic or -keto carbon (1556)	WN (—NO_2 group)-carbon on resonating ring (6927)
1	F (fluorine atom) (397) I (iodine atom) (1753)	O-two non-keto carbons (ethers) (7219)	WN, all other -NO_2 W, not in WN or WS (447)
2	M (imido —NH—) -non-carbon or -keto carbon (not in MV) (2921)	O-one carbon only (aldehydes, quinones) (1241)	WS (in sulfonic acids, sulfones, etc.) (1964)
3	MV- or MVMV-non-keto carbons only (3961)	O-others (not in OV) (1331)	S (sulfur atom) not in WS (1407)
4	M (imino —NH—) -non-keto carbons only (3780)	Q-carbon in resonating ring (phenols) (6969)	X (four-branched carbon) (1758)
5	K (quaternary nitrogen) and N-keto carbons or -non-carbon only (899)	Q-other carbon (not in QV) (alcohols, enols) (3723)	Y (three-branched carbon) (12,015)
6	N-non-keto carbon only (7201)	Q-non-carbon or ionic (2980)	Other element: B, Si, P, As, Se, Te, and all metals (2068)
7	N-one or two non-keto carbons (not in WN) (6940)	V (keto carbonyl) -carbon only (ketones) (6138)	Extra punch for CN, CNO, CNS, NUN, K, OUR, VV, WN-alkyl (3128)
8	Z (amino, —NH_2)-carbon in resonating ring (3758)	V-non-carbon (not in QV, MV, or OV) (2917)	Extra punch for F, MM, MVMV, NN, OO, SS, UU (CC) (1729)
9	Z, all other —NH_2 (amino, amido) (5087)	MV- or MVMV-non-carbon or -keto carbon (2172)	

arranged by melting point of the compound, in ascending order. Cards for compounds with melting point below zero were removed by inspection and placed in proper "reverse" order. This third arrangement was listed. The cards then were sorted back into alphabetical order by notation and refiled manually with the other cards in the V-non-carbon deck, to be ready for future searches. This last operation can be done more rapidly if a collating machine is available. Nevertheless the entire searching, sorting, listing, and refiling operation to produce these three printed lists of 199 acyl halides took only 1 hour. Obviously the 5 minutes spent in visual inspection to find -VG combinations is not a significantly large part of the total time required.

Similar lists were prepared from the 24,700 compounds for 350 semicarbazones, 600 oximes, 120 acid anhydrides, 525 amides, and smaller numbers of imides and acyl bromides, with very similar findings relative to the amount of visual inspection needed and the total preparation time required.

Searches on 50,000 Compounds

When the catalog had been expanded to 50,000 compounds, another series of searches was tried with the techniques described above and the 1000-card-per-minute sorter which had become available. A semicarbazone search, previously mentioned, produced the cards for 1097 semicarbazones in 8 minutes, with only two unwanted cards. A more complex search produced simultaneously the cards for 420 phenylhydrazones, 50 *p*-bromophenylhydrazones, 230 *p*-nitrophenylhydrazones, and 250 2,4-dinitrophenylhydrazones, each in separate alphabetized groups ready for listing, in 25 minutes of machine sorting and 55 minutes of visual inspection. As a by-product of this search, the machine-sorts to remove thiosemicarbazones (by sorting for S, column 5, punch position 3 and Z, column 3, punch position 9) and phenylsemicarbazones (by sorting for MV, column 4, punch position 9) gave "pure products" in each of these categories without "contamination" either from compounds in the four groups being sought or from other compounds.

Summary

A method has been developed for locating data about organic compounds with similar functional groups by means of punched-card techniques on a standard IBM sorting machine. By a judicious combination of machine sorting (made possible by the searching code described above) and visual inspection (made possible by the intelligible nature of the Wiswesser notation), the use of expensive and complicated machines has been avoided. The Wiswesser notation makes it possible to locate individual compounds at once in alphabetically arranged lists or files of cards. The searching system described above makes it possible to locate compounds with similar functional groups among the 50,000 organic compounds currently in the punched-card file described, and many of these searches can be completed in a matter of minutes.

Printed lists of the compounds, with the complete line-formula structure and other data, have been prepared quickly and effectively with an IBM tabulating machine from the cards located in the search. The conciseness of the Wiswesser notation makes the system efficient, since the notation and data for a given compound may be carried on a single card, which can be used in a tabulating machine to prepare lists of notations and data directly (*6*).

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6. I am grateful to the University of Hawaii, Honolulu, where this study was carried out, for a reduction in teaching load which made part of this work possible; to the College of Business Administration of the university for access to IBM equipment; and to John Ferguson and Tad Nakano for their patient help with machine problems.

Science in the News

Royal Society Celebrates Tercentenary

In 1960 the Royal Society celebrates the tercentenary of its founding. It was on 28 November 1660 that the decision was taken to form a society for the promoting of experimental philosophy, by a group of 12 remarkable men, including Lord Brouncker, Robert Boyle, Sir William Petty, and John Wilkins, who met after a lecture by Christopher Wren at Gresham College in the city of London.

Two years later, Charles II granted them a royal charter which gave the society its constitution and its name, "The Royal Society of London for Improving Natural Knowledge." Some of those who were present on foundation day had been meeting with other enthusiasts to discuss the new philosophy during the previous 15 years, first in London, then in Oxford, and later in London again, after 1658.

Oldest Scientific Society

The Royal Society is the oldest scientific society in the world with a continuous record of activity, and today it fulfills the functions of a British academy of sciences, with members drawn from most of the countries of the British Commonwealth. All the great names in British science are to be found in the annals of the society, and many of the world's most famous men of science are in the roll of foreign members. A close and friendly relationship with the scientists of other countries has been one of the features of the society from its earliest days.

Its original constitution recognized