

International Atomic Energy Agency

INDC(FR)-21/GA

INDC

INTERNATIONAL NUCLEAR DATA COMMITTEE

The "GAPHYOR" System: A Computerized Retrieval System
of the Properties of Atoms, Molecules, Gases and Plasmas

J.L. Delcroix

August 1977

IAEA NUCLEAR DATA SECTION, KÄRNTNER RING 11, A-1010 VIENNA

Reproduced by the IAEA in Austria
August 1977
77-6836

Working Paper

(Rapport L.P. no. 163)

THE "GAPHYOR" SYSTEM: A COMPUTERIZED RETRIEVAL SYSTEM
OF THE PROPERTIES OF ATOMS, MOLECULES, GASES AND PLASMAS

J.L. Delcroix

Submitted to the First Meeting of A+M Data Centres

Vienna, 9 - 13 May 1977

The "GAPHYOR" System: A Computerized Retrieval System
of the Properties of Atoms, Molecules, Gases and Plasmas

J.L. Delcroix

August 1977

SUMMARY - GAPHYOR (GAz PHYsique ORsay) is a retrieval system of the simple properties of atoms and molecules (energy levels, lifetimes, dipole moments, polarizability etc.), of the interaction properties between these particles (cross-sections, reaction rates etc.) and of the macroscopic properties of the corresponding gases (viscosity, electronic and ion mobility, thermodynamic functions etc.). The chemical systems described must be based on a small number of elements (1 to 4 in the most recent version) and composed of molecules having 8 atoms at the most. In the present article the fundamental principles of GAPHYOR are described and by means of a few simple statistics the present state of the bank after five years of operation is analysed. On 1.11.76 the file contained more than 33,000 lines, and these increase by about 10,000 per year. The information comes from about 300 periodicals, although 45% of the results are taken from 4 principal journals. Geographical analysis of the file provides useful information about the scientific work of the various research centres and the scientific publishing policies of the different countries. Finally, the qualities, difficulties and possible improvements of GAPHYOR are analysed.

1. INTRODUCTION

The basic properties of single atoms or molecules (energy levels, lifetimes of excited states, etc.), the properties of interaction between such particles (cross-sections for various collision processes etc.) and certain basic macroscopic properties (transport coefficients, etc.) are the fundamental data of the physics of gases. This set of data is complex and constantly undergoing change. In the present report the work done at the Orsay Plasma Physics Laboratory is described for purposes of classification and analysis of the data in question, and a classification method which permits the handling of bibliographical information by computer is proposed.

The system which has evolved is called "GAPHYOR" (GAz - PHYsique - ORsay). It is in effect a computer-based data bank for documentation. Conceived in broad outline at the beginning of 1972, GAPHYOR was initially tried out at the laboratory level. Early in 1973, it was offered as a specialized documentation service for users in France. In 1975, the service was extended to users in other countries.

2. DEMARCATION OF THE FIELD

The approach has been to select and classify data from the standpoint of a specific group of users - physicists, physical chemists and engineers concerned with atomic and molecular physics and the physics of neutral or ionized gases under conditions of temperature and pressure attainable on Earth. Therefore no attempt has been made to meet the needs of nuclear physicists interested in very high energies or of chemists studying complex molecules. More precisely, the approach has been to limit the field studied according to the following guidelines:

- Only systems based on a small number of chemical elements are studied. In its 1972 version, GAPHYOR only included systems based on a chemical element X or two elements X and Y. For example, it covered the properties of N_2 (1 element),

or of the mixtures $N_2 - O_2$, $NO - N_2 - O_2$ (2 elements), but not those of CH_3OH or of the mixture $N_2 - CO_2$ (3 elements). The elimination of systems with more than two elements seemed essential for the compilation of data lists of reasonable size. However, in practice this limitation proved too restrictive and, more recently, the extension of GAPHYOR to 3-element (GAPHYOR 3) and 4-element (GAPHYOR 4) systems has been studied. Moreover, an a posteriori statistical analysis influenced the decision: Figure 1 shows that GAPHYOR 3 contains a large proportion of useful information, that GAPHYOR 4 contains very little and that GAPHYOR 5 hardly exists at all. The statistics appearing in Fig. 1 are based on a rather restricted number of samples. They must be considered only as a first step. Especially the ascending arrows stress the fact that GAPHYOR 3 and 4 are possibly underestimated in this figure. Anyway this modification appears not so important as to change qualitatively the conclusions on the faible importance of GAPHYOR 4 and moreover GAPHYOR 5. In view of these conditions it was decided to set up GAPHYOR 3, which has been in operation since early 1976, and GAPHYOR 4, which will come into operation in 1977.

- In the systems defined above only the properties of "small" molecules (or ions) containing at the most 8 atoms are studied. Therefore the properties of NH_3 , CH_4 and SF_6 are described, but not those of benzene. However, in order to help certain users, an element in the code has been provided which makes it possible to show which publications deal with larger molecules.
- As far as the energies involved are concerned, a maximum of 10 keV (in the centre-of-mass system) has been taken as a limit. In other words, references which only contain information relating to energies above 10 keV have been eliminated. This does not mean that our lists contain no information in this energy range since numerous publications contain information straddling this limit (these are shown by a special code letter).

- With regard to low energies, no lower limit has, of course, been fixed. As this is the field which most interests physicists and physical chemists working on gases, a special code letter for references below 10 eV has been provided.

3. SCANNING OF JOURNALS AND BOOKS

With due regard to the field as defined above and the facilities available, the scientific press is scanned in two stages: about 30 journals which seem to us to be the most important^{1/} are analysed as soon as they come out. A list of them is shown below in Table 3.

Also the following documents are scanned systematically:

Conference proceedings;

Reference books;

and in a less systematic fashion the following documents:

Internal laboratory reports;

French theses.

Finally, we obtain a wider overall view by using section 165 of the Abstracts Bulletin of the National Scientific Research Centre (C.N.R.S.).

^{1/} The choice of these journals is in fact influenced by an a posteriori statistical analysis of the contents of the file as presented in Table 3.

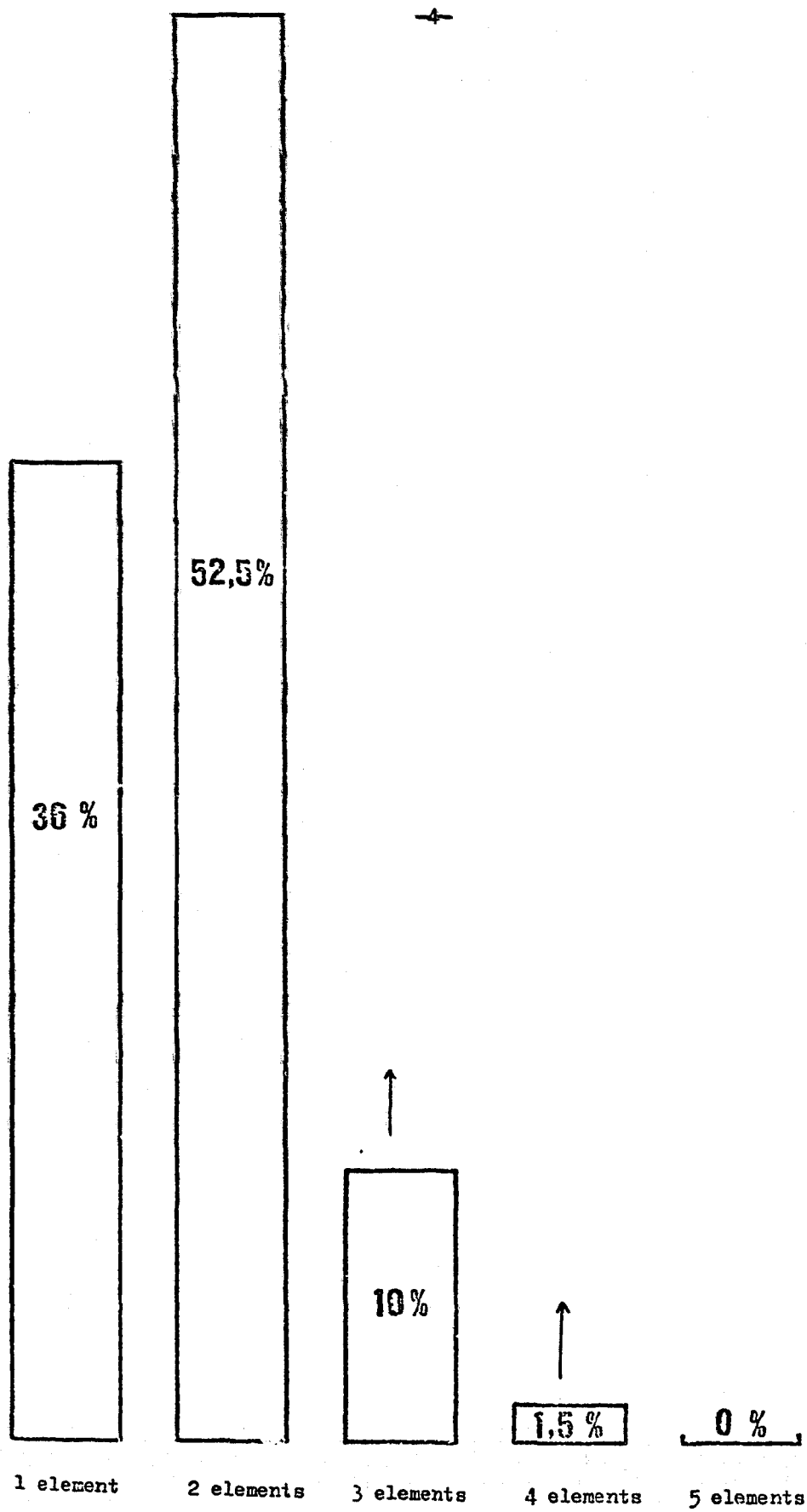


Figure 1

From each reference we make up one or more "computer lines". Each of these lines is composed of a set of "descriptors" and recorded in the computer memory. All these "computer lines" together make up the "GAPTOR" file.

4. DESCRIPTION OF A COMPUTER LINE

4.1. Descriptors carried by a computer line

Each computer line carries the following descriptors:

(a) Archive descriptor:

Entry number

(b) Classification descriptors:

| | | |
|---|--------------------------|--------------------|
| Families A, B, C and D | | (D ₁) |
| Category K | | (D ₂) |
| Molecule P indices (subscripts/superscripts) | l m n p, i x | (D ₃) |
| Molecule Q indices (subscripts/superscripts) | l' m' n' p', i' x' | (D ₄) |
| Molecule R indices (subscripts/superscripts) | l'' m'' n'' p'', i'' x'' | (D ₅) |
| Simplified description | | (D ₆) |
| Molecule S indices (subscripts/superscripts) | r s t u, j y | (D ₇) |
| Molecule T indices (subscripts/superscripts) | r' s' t' u', j' y' | (D ₈) |
| Molecule U indices (subscripts/superscripts) | r'' s'' t'' u'', j'' y'' | (D ₉) |
| Year of publication | | (D ₁₀) |

(c) Information and filtering descriptors

Experimental order V

Experimental order W

Elements concerned X, Y, Z and Z'

Marginal and qualitative descriptors

(d) Localization descriptors

- Journal ("Revue")
- Volume ("Tome")
- Page ("Page")
- Author ("Auteur")
- Country ("Nation")
- Province ("Province")
- City ("Cité")

The set of these descriptors can be represented by the following formula:

$$F = \underline{A}, \underline{B}, \underline{C}, \underline{D/X}, Y, Z, Z'/\underline{K/P}, \underline{Q}, \underline{R/V/DS/S}, \underline{T}, \underline{U/W/}$$
$$/\underline{REV}, \underline{TOM}, \underline{PAG}, \underline{AUT/ANN/NA}, \underline{PR}, \underline{CI/QUAL/NUM/}$$

in which classification descriptors are underlined. A more detailed analysis of each of these descriptors is given below.

4.2. Mendeleev families (A, B)

All the processes concerned relate to a chemical system with one element X, two elements X and Y, three elements X, Y, Z or four elements X, Y, Z and Z'. Initial classification of the data is based not on the particular elements concerned but on the Mendeleev families to which they belong. These families are designated by A, B, C, D. This approach simplifies classification because very often a given author is studying in a given publication the properties of all the elements X of one family A with respect to a certain process. In other words, the whole set of 92 x 91 x 90 x 89 combinations X, Y, Z, Z' can be brought together using the Mendeleev families into a more manageable set of combinations A, B, C and D, which is well adapted to actual needs. After a few experiments we therefore decided to classify the elements into families according to the following list:

| | |
|----|------------------------------|
| R | He Ne Ar Kr Xe Rn |
| H | H |
| 1A | Li Na K Rb Cs Fr |
| 1B | Cu Ag Au |
| 2A | Be Mg Ca Sr Ba Ra |
| 2B | Zn Cd Hg |
| 3A | B Al Ga In Tl |
| 3B | Sc Y La Lu |
| 4A | C Si Ge Sn Pb |
| 4B | Ti Zr Hf |
| 5A | N P As Sb Bi |
| 5B | V Nb Ta |
| 6A | O S Se Te Po |
| 6B | Cr Mo W |
| 7A | F Cl Br I At |
| 7B | Mn Te Re |
| 8A | Fe Co Ni |
| 8B | Ru Rh Pd |
| 8C | Os Ir Pt |
| 9A | Ce Pr Nd Pm Sm |
| 9B | Eu Gd Tb Dy Ho |
| 9C | Er Tm Yb Lu |
| 9D | Th Pa U Np Pu |
| 10 | general articles (see below) |

It can be seen that the elements are in this way classified more or less in order of electro-positive valence (from 0 to 7), and within a single family in order of their atomic masses. For convenience the "triads", rare-earth elements and actinides have been placed in positions 8 and 9.

The order thus defined can be considered as a ranking order and the expressions

$A < B$

$X < Y$

mean that family A comes before family B in this order, and similarly for X and Y (for example: $H < 1A$, $4B < 5A$, $Li < Na$, etc.).

In general terms, a group of 4 families will always be written

A B C D

on the assumption that

$A \leq B \leq C \leq D$

Groups of less than 4 families are written by inserting zeroes on the right as follows:

A, B, C, 0

A, B, 0, 0

A, 0, 0, 0

Using these writing rules, the two groups A B C D and A', B', C', D' will be classified in the order

$A B C D < A' B' C' D'$

if one of the following conditions is fulfilled:

$A < A'$

$A = A', B < B'$

$A = A', B = B', C < C'$

$A = A', B = B', C = C' = D < D'$

Where the 0 is the first of the families, so that one has for example:

$A, B, C, 0 < A B C D$

Finally, in the bibliography, we sometimes find publications treating a specific process but without being limited to a specific chemical system (synthetic articles, theoretical studies, etc.). These are to be classified by introducing the "family" .0 which can be combined with all the others to form groups such as 10-0-0-0, 10-10-0-0, 10-10-10-0, R-10-0-0 etc.

4.3. Process categories (K)

In the same way that the elements are grouped in families, the process involved is rapidly identified by the "process category" descriptor K. The categories considered are:

1. Properties of atoms and molecules;
2. Photon collisions;

3. Electron collisions;
4. Atom-atom, atom-molecule and molecule-molecule collisions
(including the corresponding ions);
5. Macroscopic processes.

4.4. Description of the process

4.4.1. Initial state (P,Q,R)

The process under consideration is normally identified by the following code letters:

P, Q, R/S, T, U

In the case of collisions between particles (process categories 2-4) the above is the classical method in collision physics of writing down the reaction:



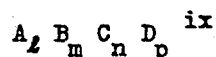
P, Q, R signify the initial state and S, T, U the final state. By convention this notation will be extended to two other process categories, according to rules that will be described later. Therefore, in general, the "initial" state will be described as follows:

P, Q, R/ - for a problem involving 3 bodies;

P, Q/ - for a problem involving 2 bodies;

P/ - for a problem involving 1 body.

The symbols P, Q and R may represent a photon, an electron or, more generally, an atom or molecule of the A - B - C - D system which may be ionized and/or excited:



The subscripts l, m, n and p thus define the empirical formula of the molecule while the superscripts i and x show (using the following conventions), the ionization and excitation states of the molecule as appropriate:

i = superscript denoting ionization

i = 0 neutral atom or molecule

i = 1 positive ion with 1 charge

i = 2 positive ion with 2 charges

i = 5 positive ion with more than 4 charges^{2/}

i = 6 negative ion with 1 charge

i = 7 negative ion with 2 charges

i = 9 inner shell ionized atom or molecule

x = superscript denoting excitation

x = 0 ground state

x = 1 rotational excitation (r)

x = 2 vibrational excitation (v)

x = 3 electron excitation (*)

x = 4 oriented atom or molecule (s)

x = 5 excitation (* r)

x = 6 excitation (* v)

x = 7 excitation (* s)

x = 8 excitation (r v)

x = 9 excitation (* r v)

In conjunction with this system the following rules are used for purposes of ranking the various bodies that make up the initial state:

Generally, in the case of a collision between three heavy particles the initial state P, Q, R will be written as follows:

$$A_l B_m C_n D_p^{ix}, A_l' B_m' C_n' D_p^{i'x'}, A_l'' B_m'' C_n'' D_p^{i''x''}$$

two molecules being written in the following order:

$$A_l B_m C_n D_p^{ix} < A_l' B_m' C_n' D_p^{i'x'} \quad (1)$$

if one of the following conditions is met:

^{2/} With respect to positive ions with more than 4 charges, the exact state of charge is shown by the use, as an exception, of the superscripts i'' and x''.

$$p < p' \quad (2)$$

$$p = p', n < n' \quad (3)$$

$$p = p', n = n', m < m' \quad (4)$$

$$p = p', n = n', m = m', l > l' \text{ (N.B.!) } \quad (5)$$

$$p = p', n = n', m = m', l = l', i > i' \quad (6)$$

$$p = p', n = n', m = m', l = l', i = i', x > x' \quad (7)$$

- Where one or two of the particles involved are light particles (photons or electrons) they are considered to correspond to $l = m = n = p = 0$, and are written in first place in the P,Q positions beginning with the photon;
- In problems involving two bodies it is assumed that $R = 0$ and the particles are ranked in the order P,Q according to the same rules as for problems involving three bodies (formulae (2) to (7));
- In problems involving one body, $Q = R = 0$ is assumed;
- These rules make it possible in general to write the initial state P,Q,R in an unequivocal way. However, there are possible cases of ambiguity: where two of the families A,B,C,D considered are identical. The special rules concerning these cases are discussed in Reference [4].

It may happen in certain cases that ranking order P,Q,R defined by the preceding rules is ill suited to the experimental conditions involved. For example, in charge exchange collisions most experiments are made with a beam of fast particles which play a special role and which it is therefore logical to write in the initial position, even though according to rules (2) to (7) these particles should possibly occupy position Q or R. In these circumstances the bodies will nevertheless be written in the order P,Q,R as defined by formulae (2) to (7), but the different order (e.g. Q,P,R) that is best suited to the experimental situation will be indicated by the code sign V using the following conventions:

$$V = 0 \text{ (PQR) , } 1 \text{ (QPR) , } 2 \text{ (PRQ) , } 3 \text{ (RPQ) , } 4 \text{ (QRP) , } 5 \text{ (RQP)}$$

4.4.2. Final state: detailed description (S,T,U)

In process categories 2-6 (collisions) the final state, if it is known completely, is indicated according to the same rules as the initial state, as follows:

$$\begin{array}{c} A_r \ B_s \ C_t \ D_u^{jy} < A_r' \ B_s' \ C_t' \ D_u'^{j'y'} < A_r'' \ B_s'' \ C_t'' \ D_u''^{j''y''} \\ S \qquad \qquad \qquad T \qquad \qquad \qquad U \end{array}$$

The rules for ranking S,T,U are the same as for P,Q,R; if an "experimental" order is preferred, this is indicated by the descriptor W. With: W = 0 (STU), 1 (TSU), 2 (SUT), 3 (UST), 4 (TUS), 5 (UTS).

If the final state involves more than three particles they are ranked according to the same rules and only the last three are written.

If the final state is only partially known, only the bodies actually known are to be written, beginning with S and leaving blank the unknown bodies.

4.4.3. Final state: simplified description (D S)

In the case of some collision processes, such as elastic collision or symmetric charge transfer, there is no need to describe the final state in detail. In other cases, the process in question is a superposition of several elementary processes resulting in different final states. Lastly, in process categories 1 and 5 the very concept of a final state loses all meaning.

For dealing with these cases a simplified description of the process is introduced - an abbreviation consisting of two code letters. (Appendix B contains a list of the abbreviations used in each process category).

Since the concept of the final state lacks all meaning in categories 1 and 5, the code is used in the following way:

DS is a substantive

S, T, U are complements

Example: DS = MI S = H₂O⁺ → mobility of H₂O⁺ ions.

5. ELEMENTS CONCERNED (X, Y, Z, Z')

The Mendeleev families (A, B, C, D) relating to a given publication having been indicated, it should be stated which elements of these families are concerned; this is done by means of the descriptors X, Y, Z, Z'.

These can have the values 1, 2, 3, 4, 5, 6, where the figures 1, 2, 3, 4, 5, 6 denote the rank of an element in the family under discussion.

6. MARGINAL AND QUALITATIVE DESCRIPTORS (QUAL)

Marginal and qualitative descriptors are as follows:

- M (molecules) means publications dealing with systems containing molecules with more than eight atoms.
- H (high energies) means publications describing collision processes in the energy range above 10 keV (in the centre-of-mass system).
- L (low energy) means publications describing collision processes in the energy range below 10 eV (in the centre-of-mass system).
- N (nucleus) means publications involving isotopic effects.
- E, T mean publications containing work with an experimental or a theoretical bias, while S means review articles.
- Finally, it should be said that certain special conventions have proved useful during experiments with the system. These conventions, which are sometimes exceptions to the overall code, are described in Ref. [3].

7. BIBLIOGRAPHICAL REFERENCES (REV, TOM, PAG, AUT)

The title of the journal, the volume, the page, the first author and the year of publication are written in code language according to the following scheme:

| REV | TOM | PAG | AUT | AN |
|-------|-------|---------|-----------------|-------|
| 7 0 | 2 2 | 1 3 4 1 | D U P O N T J L | 7 4 |
| _____ | _____ | _____ | _____ | _____ |

For this the main journals have been classified according to a code [1] composed of 2 digits for the more common of them, 3 or 4 digits for the others (e.g. "70" means "Physical Review A").

The sign 00 placed in position REV means Conference Proceedings and 97 reviews in book form. The list of these works constitutes an annexed file [1]; the corresponding references are indicated where necessary in position TOM in the place of the volume number. Similarly, the signs 98 and 99 placed in position REV mean laboratory reports and theses: the lab or the place of dissertation is reported instead of the volume according to a code [1].

8. GEOGRAPHY OF LABORATORIES

The above bibliographical references do not always give exact information on where a given "GAPHYOR" result has been obtained. It often happens in fact that a researcher working in a given country A publishes his results in a journal appearing in another country B.

For this reason we have specified the geographical location of the laboratory where work mentioned in a publication has been carried out, by means of a three-stage code:

| | |
|----------|-------------------|
| Nation | <u>U</u> <u>S</u> |
| Province | <u>M</u> <u>A</u> |
| Cité | <u>C</u> <u>A</u> |

where the above example means United States, Massachusetts, Cambridge. A geographical code of countries, provinces and cities [2] has been drawn up. This code is unequivocal in the sense that, for example, two different towns in the same province are shown by two different abbreviations. When the publication concerned mentions several places where the work has been carried out, the one shown in GAPHYOR corresponds to the address of the first author.

9. STORAGE IN THE FILE

Storage in the file is effected by using the classification descriptors according to a hierarchy corresponding to the order in which we have written them. In other words, two lines F and F' characterized by the descriptors D_1, D_2, \dots, D_{10} and $D'_1, D'_2, \dots, D'_{10}$ will be classified in the order

F before F'

if one of the following conditions is fulfilled:

$$\begin{aligned} D_1 &< D'_1 \\ D_1 &= D'_1 \text{ and } D_2 < D'_2 \\ D_1 &= D'_1 \quad D_2 = D'_2 \text{ and } D_3 < D'_3 \\ &\dots\dots\dots \end{aligned}$$

As a last resort, if their 10 classification descriptors are the same, the lines F and F' are ranked according to entry number. For these classification rules to be applied, an ordering of the values for each of the descriptors D_1 to D_{10} must therefore be established. For the descriptors $D_2, D_3, D_4, D_5, D_7, D_8, D_9, D_{10}$ which have been coded in a numerical form, this is simple: their values are ranked according to the natural order of whole numbers^{3/} (for this ranking it is to be understood that a blank space comes before a zero).

For the descriptor D_1 a ranking order has been worked out from the list of Mendeleev families as we have seen in section 4.2.

Finally, the ranking of the values of descriptor D_6 must be established for each process category: the order chosen is that which appears in Appendix A. Apart from this it is accepted that when this descriptor is not specified (D S spaces left blank), this corresponds to an infinite value of D_6 . In other words, the lines where this descriptor is not shown are classified after all those on which it is.

^{3/} When a photon (P) or electron (E) is involved it has been agreed that $P < E < 0$.

10. RETRIEVAL FROM THE FILE

Retrieval is effected by specifying the classification descriptors D_1 to D_{10} with, if required, selection based on the filtering descriptors. For this it is necessary only to fill in an order form. On the form, the "client" fills in the non-coded part and we translate the information into code language. The computer responds by printing a list of references relating to the phenomena thus specified. If the client wants fairly extensive information, he writes only the first descriptors (e.g. D_1 and D_2). The computer then provides a set of references ranked on the basis of the established GAPHYOR ordering, i.e. according to the values of the descriptors left free ($D_3, D_4 \dots, D_{10}$ in the example chosen). The list obtained is sent to the client with a simple explanation of the code used. As an example we show here the result of a question on nitrogen - zinc, cadmium, mercury systems (publication years 1970-75).

11. STATISTICAL ANALYSIS OF THE GAPHYOR FILE

11.1. Theoretical volume of the GAPHYOR file

It is useful to calculate the theoretical volume of the GAPHYOR file, i.e. the number of spaces it contains, a space being defined by a series of values taken by the descriptors D_1 to D_{10} . A simple combinatory analysis calculation [Appendix A] shows an enormous number, of the order of:

| | |
|---------------------|------------------------|
| $4 \cdot 10^{15}$ | cases for "GRAPHYOR" 1 |
| $1,5 \cdot 10^{20}$ | " " "GRAPHYOR" 2 |
| 10^{24} | " " "GRAPHYOR" 3 |
| $1,5 \cdot 10^{27}$ | " " "GRAPHYOR" 4 |

The number of lines actually contained in GAPHYOR on 1.11.1976 was about 33,000 and is increasing by about 10,000 lines per year. It can be seen how few of the spaces in the file are filled.

11.2. Years of publication

Statistical analysis by years of publication is shown in Table 1 which calls for the following remarks:

The sharp increase between 1969 and 1970 reflects the launching of GAPHYOR in 1970; the lines previous to 1970 only represented a partial scanning of the literature;

| FAMILIES | | | | | | | | | | RCD | | | ELEMENTS MENTIONED | | | JOUR- | VOL. | PAGE | AUTHOR | MARGIN | GEOGRAPHY | | | |
|----------|----|----|---|----|----|----|----|----|---|-----|----|-------|--------------------|---|---|-------|------|------|-------------|--------|-----------|-----|----|----|
| AA | BB | CC | P | P | Q | R | SI | S | T | U | YR | NUM | X | Y | Z | NAL | | | | DESCR | V | COU | PR | CI |
| 281 | 5A | 1 | 1 | 2 | C6 | | EN | | | | 73 | 9619 | 3 | | | 48 | 45 | 732 | HAUSZ | | | | | |
| 281 | 5A | 4 | 1 | C | CC | 01 | GO | | | | 72 | 5233 | 3 | 1 | | 16 | 50 | 1928 | WJUNGAAR | H | E | | | |
| 281 | 5A | 4 | 1 | C | CC | 01 | OC | | | | 72 | 5234 | 3 | 1 | | 16 | 50 | 1928 | WJUNGAAR | H | E | | | |
| 281 | 5A | 4 | 1 | C | CC | 01 | 1C | | | | 73 | 7662 | 3 | 1 | | 70 | 7 | 9319 | WJUNGAAR | H | AE | | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | C | | | | 74 | 15504 | 3 | 1 | | CC | 60 | 106 | BURNHAM R | T | L | E | | |
| 281 | 5A | 4 | 1 | C | 03 | 02 | O | | | | 74 | 17243 | 3 | 1 | | 28 | 35 | 952 | LANIEPCE B | | L | E | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | O | | | | 74 | 17562 | 3 | 1 | | 28 | 35 | 941 | LANAYE B | | L | AE | | |
| 281 | 5A | 4 | 1 | C | 02 | 02 | O | | | | 74 | 17954 | 2 | 1 | | 16 | 52 | 2228 | ICZAJKOWSKI | | L | E | | |
| 281 | 5A | 4 | 1 | C | 03 | 02 | O | | | | 74 | 18153 | 3 | 1 | | 30 | 61 | 5158 | BURNHAM R | T | L | E | | |
| 281 | 5A | 4 | 1 | 0 | 03 | 02 | O | | | | 75 | 32361 | 2 | 1 | | 20 | 29 | 421 | BRECKENRID | T | L | AE | US | UT |
| 281 | 5A | 4 | 1 | C | 03 | 02 | O | | | | 75 | 30016 | 3 | 2 | | 20 | 31 | 577 | HAUSE H F | | L | E | US | TN |
| 281 | 5A | 4 | 1 | C | C3 | 02 | O | | | | 74 | 15505 | 3 | 1 | | CC | 60 | 106 | BURNHAM R | T | L | E | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | O | | | | 74 | 17242 | 3 | 1 | | 28 | 35 | 952 | LANIEPCE B | | L | E | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | O | | | | 74 | 18154 | 3 | 1 | | 30 | 61 | 5158 | BURNHAM R | T | L | E | | |
| 281 | 5A | 4 | 1 | C | 03 | 02 | C3 | | | | 72 | 21242 | 3 | 1 | | 57 | 70 | 601 | LANPE F W | T | AS | | | |
| 281 | 5A | 4 | 1 | C | CC | 02 | C3 | | | | 70 | 3709 | 3 | 1 | | 20 | 5 | 128 | CALLEAR A | | L | E | | |
| 281 | 5A | 4 | 1 | C | 00 | 02 | C3 | | | | 73 | 11170 | 3 | 1 | | 44 | 77 | 875 | MADHAVAN V | TM | L | AE | | |
| 281 | 5A | 4 | 1 | C | 03 | 02 | C | | | | 71 | 4387 | 3 | 1 | | 123 | 44 | 123 | MORIGLCHI | T | L | E | | |
| 281 | 5A | 4 | 1 | C | 02 | 02 | C | | | | 72 | 6755 | 3 | 1 | | 70 | 6 | 2101 | PIRE J | | L | E | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | C | | | | 72 | 6757 | 2 | 1 | | 28 | 33 | 652 | LANIEPCE B | | L | E | | |
| 281 | 5A | 4 | 1 | C | 02 | 02 | O | | | | 72 | 72701 | 1 | 1 | | 22 | 275 | 187 | CRIMER G | | E | | | |
| 281 | 5A | 4 | 1 | C | 02 | 02 | O | | | | 73 | 9988 | 3 | 1 | | 88 | 69 | 57 | CALLEAR A | T | L | E | | |
| 281 | 5A | 4 | 1 | C | 03 | 02 | O | | | | 73 | 11173 | 3 | 1 | | 44 | 77 | 875 | MADHAVAN V | TM | L | AE | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | C | | | | 70 | 266 | 3 | 1 | | 20 | 6 | 47 | CALLEAR A | | L | E | | |
| 281 | 5A | 4 | 1 | C | 02 | 02 | O | | | | 73 | 11168 | 3 | 1 | | 44 | 77 | 875 | MADHAVAN V | TM | L | AE | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | O | | | | 71 | 4388 | 3 | 1 | | 123 | 44 | 123 | MORIGLCHI | T | L | E | | |
| 281 | 5A | 4 | 1 | C | 02 | 02 | O | | | | 72 | 6754 | 3 | 1 | | 70 | 6 | 2101 | PIRE J | | L | E | | |
| 281 | 5A | 4 | 1 | C | C3 | 02 | O | | | | 72 | 6756 | 2 | 1 | | 28 | 33 | 652 | LANIEPCE B | | L | E | | |
| 281 | 5A | 4 | 1 | C | 02 | 02 | O | | | | 72 | 8045 | 3 | 1 | | 70 | 7 | 1442 | PIRE J | | L | E | | |
| 281 | 5A | 4 | 1 | C | 03 | 02 | C | | | | 73 | 11167 | 3 | 1 | | 44 | 77 | 875 | MADHAVAN V | TM | L | AE | | |
| 281 | 5A | 4 | 1 | 0 | 02 | 10 | CO | 02 | C | | 73 | 10613 | 3 | 1 | | 70 | 8 | 256 | PHANELE R | | L | E | | |
| 281 | 5A | 4 | 1 | C | 0 | 02 | C | | | | 70 | 342 | 2 | 1 | | 28 | 31 | 145 | LANIEPCE B | | E | | | |
| 281 | 5A | 4 | 1 | 0 | C7 | 02 | C | | | | 72 | 7271 | 1 | 1 | | 22 | 275 | 187 | CRIMER G | | E | | | |
| 281 | 5A | 4 | 1 | C | C7 | 02 | C | | | | 73 | 7665 | 3 | 1 | | 16 | 51 | 724 | PHANELE R | | L | E | | |
| 281 | 5A | 4 | 1 | C | C7 | 02 | C | | | | 74 | 19859 | 3 | 1 | | 90 | 29 | 661 | BALMANN M | T | L | E | DB | TU |
| 281 | 5A | 4 | 1 | 2C | CC | 01 | C7 | | | | 70 | 2346 | 2 | 1 | | 28 | 31 | 145 | LANIEPCE B | | L | E | | |
| 281 | 5A | 4 | 1 | 2C | 02 | 02 | C | | | | 73 | 10614 | 3 | 1 | | 70 | 8 | 256 | PHANELE R | | L | E | | |
| 281 | 5A | 5 | 1 | C2 | | | | | | | 71 | 4767 | 3 | 1 | | 684 | 4 | 11 | STRUMIA F | | E | | | |
| 281 | 5A | 5 | 1 | C | | | | | | | 73 | 9971 | 3 | 1 | | 30 | 59 | 582 | GOLDSTEIN | | E | | | |
| 281 | 5A | 5 | 1 | 0 | | | | | | | 73 | 10612 | 3 | 1 | | 70 | 8 | 256 | PHANELE R | | L | E | | |

GAPHYOR DATA BANK

PAGE 1. END OF CARD INDEX 40 ENTRIES.

RETRIEVAL SPECIMEN: Nitrogen - zino, cadmium, mercury systems.

TABLE 1 - Statistics by year of publication (on 1.11.1976)

| YEAR | NUMBER OF CARDS | Z |
|--------|-----------------|------|
| < 1968 | 3376 | 10,0 |
| 1968 | 457 | 1,4 |
| 1969 | 705 | 2,1 |
| 1970 | 1745 | 5,2 |
| 1971 | 2443 | 7,2 |
| 1972 | 3812 | 11,3 |
| 1973 | 5483 | 16,2 |
| 1974 | 7428 | 22,0 |
| 1975 | 8118 | 24,0 |

TABLE 2 - Statistics by process categories (on 1.11.1976)

| K | NUMBER OF CARDS | Z |
|---|-----------------|------|
| Properties of atoms and molecules | 14.388 | 42,7 |
| Photon collisions | 2.490 | 7,4 |
| Electron collisions | 3.898 | 11,6 |
| Collisions between atoms and/or molecules | 8.917 | 26,5 |
| Macroscopic properties of gases | 3.944 | 11,7 |

The progressive increase between 1970 and 1974 is due to the refinement of our scanning methods rather than to an increase in scientific work. A more detailed analysis should be undertaken with the aim of better understanding the influence of these two factors.

On 1.11.1976 the scanning of the third trimester of 1975 was complete. An effort must be made to accelerate scanning and acquisition by the file. This seems possible by making scanning techniques more systematic. Since 1975 we have been updating the file quarterly so that articles that appear in months n to $n + 3$ should shortly be included in the file by month $n + 6$ or $n + 7$. Conversely, it should be pointed out that the launching of GAPHYOR 3 and 4, on which we are at present engaged, is tending to retard the scanning process.

11.3. Process categories

Statistical analysis by process category is shown in Table 2. It can be seen that GAPHYOR, originally conceived as a retrieval system for the physics of gases, is becoming more and more a retrieval system for atomic and molecular physics.

11.4. Mendeleev families

Statistical analysis by Mendeleev family is shown in Fig. 2. It can be seen that the most studied systems are, as is to be expected:

In GAPHYOR 1 (1 element system):

Rare gases

Hydrogen

Oxygen

Nitrogen

In GAPHYOR 2 (2 element systems):

Carbon - oxygen (CO , CO_2 , etc.)

Nitrogen - oxygen ($\text{N}_2 + \text{O}_2$, NO , N_2O , etc.)

Hydrogen - oxygen ($\text{H}_2 + \text{O}_2$, H_2O , etc.)

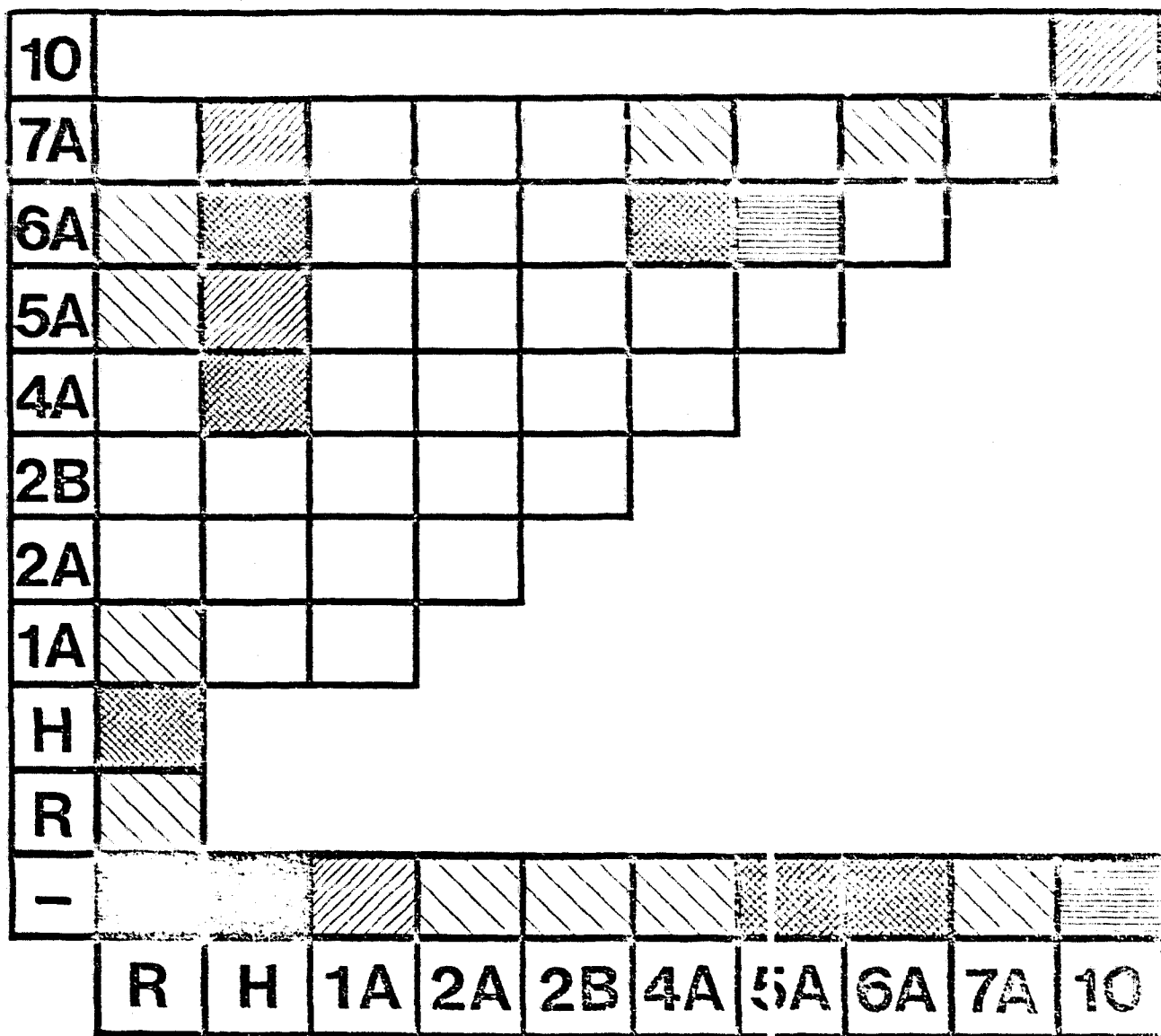


Fig. 2

Hydrogen - carbon (hydrocarbons, etc.)

Rare gases -- hydrogen

There are as yet no statistics for GAPHYOR 3 and 4.

11.5. Scientific journals

Statistical analysis by journal is shown in Table 3.

In the column entitled "Scanning method" the following symbols are used:

- + Direct scanning
- (+) Direct but not systematic scanning
- Indirect scanning from the Abstracts Bulletin of the National Scientific Research Centre (C.N.R.S.)
- + Indirect scanning until 1975, direct from 1976.

Analysis of this table shows that:

- 50 % of the information is obtained by scanning only the four most important journals and conference proceedings;
- To obtain 72% of the information, books, theses and 12 other journals must be included;
- The 21 journals which follow provide only 13 % of information;
- The last portion of information (15 %) is scattered over all the other journals (about 300 in the present state of the file).

Figure 3 shows these same results in a graphic form; this statistical information is very useful for studying possible ways of perfecting the GAPHYOR system.

11.6. Geography of laboratories

11.6.1. Statistics by countries

The statistics by journals that we have just described do not give any exact information on the countries from which material contained in GAPHYOR was obtained. It frequently happens that a researcher working in a given country A publishes his results in a journal appearing in another country B. In order to analyse in detail the

TABLE 3 Statistics by journal (on 1.11.1976)

| | JOURNAL | Scanning. method | Number of cards | Z |
|----|-----------------------------------|---------------------|--------------------|------|
| 1 | Journal of chemical physics | + | 6.443 | 19,1 |
| 2 | Physical Review A | + | 3.322 | 9,9 |
| 3 | Conférences | + | 2.865 | 8,5 |
| 4 | Journal of physics B | + | 2.523 | 7,5 |
| 5 | Chemical physics letters | + | 1.930 | 5,7 |
| | $\Sigma =$ | | 17.083 | 50,7 |
| 6 | Ouvrages | (+) | 1.029 | 3,1 |
| 7 | Molecular physics | + | 597 | 1,8 |
| 8 | Optics and spectroscopy | + | 587 | 1,7 |
| 9 | Internat. J. mass spec. ion phys. | + | 576 | 1,7 |
| 10 | J. of molecular spectroscopy | + | 571 | 1,7 |
| 11 | Thèses (françaises) | (+) | 556 | 1,7 |
| 12 | J. of quant. spect. rad. transf. | + | 484 | 1,4 |
| 13 | Physica | + | 450 | 1,3 |
| 14 | Theor. chem. acta | + | 420 | 1,2 |
| 15 | Rapports | (+) | 419 | 1,2 |
| 16 | Phys. lett. A | + | 416 | 1,2 |
| 17 | Phys. rev. lett. | + | 407 | 1,2 |
| 18 | J. of phys. chem. ref. data | + | 400 | 1,2 |
| 19 | Canad. J. of physics | + | 394 | 1,2 |
| 20 | Chemical physics | + | 394 | 1,2 |
| | $\Sigma =$ | | 24.783 | 73,5 |
| 21 | Z. für phys. A | + | 388 | 1,2 |
| 22 | Z. naturforschung A | + | 382 | 1,1 |
| 23 | Atom. and nuclear data | + | 341 | 1,0 |
| 24 | J. of the opt. soc. of Amer. | + | 325 | 1,0 |
| 25 | J.E.T.P. | + | 310 | 0,9 |
| 26 | J. chem. soc. Faraday II | + | 292 | 0,9 |
| 27 | Proc. Roy. Soc. A | - + | 217 | 0,6 |
| 28 | Comptes-Rendus B | + | 196 | 0,6 |
| 29 | J. de physique | + | 192 | 0,6 |
| 30 | J. chem. soc. Faraday Trans. I | + | 177 | 0,5 |
| | $\Sigma =$ | | 27.603 | 81,9 |

TABLE 3 - Statistics by journal (continued)

| | JOURNAL | Scanning method | Number of cards | % |
|----|-----------------------------------|--------------------|--------------------|------|
| 31 | Physica scripta | - + | 177 | 0,5 |
| 32 | J. of the phys. soc. Jap. | + | 167 | 0,5 |
| 33 | J. of mol. struct. | - + | 151 | 0,5 |
| 34 | J. of electron spec. relat. phen. | - + | 140 | 0,4 |
| 35 | J. of phys. chem. | - + | 139 | 0,4 |
| 36 | Astrophys. J. | - | 130 | 0,4 |
| 37 | Sov. phys. techn. phys. | + | 130 | 0,4 |
| 38 | Ber. Bunsengesellsch. phys. | - + | 128 | 0,4 |
| 39 | Philes. mag. | - | 107 | 0,3 |
| 40 | Int. J. quant. chem. | - | 103 | 0,3 |
| | ----- | | | |
| 50 | Faraday discussions. Chem. soc. | - + | 85 | 0,3 |
| | $\Sigma =$ | | 29.060 | 86,3 |
| | Divers | | 4.622 | 13,7 |
| | $\Sigma \Sigma =$ | | 33.682 | |

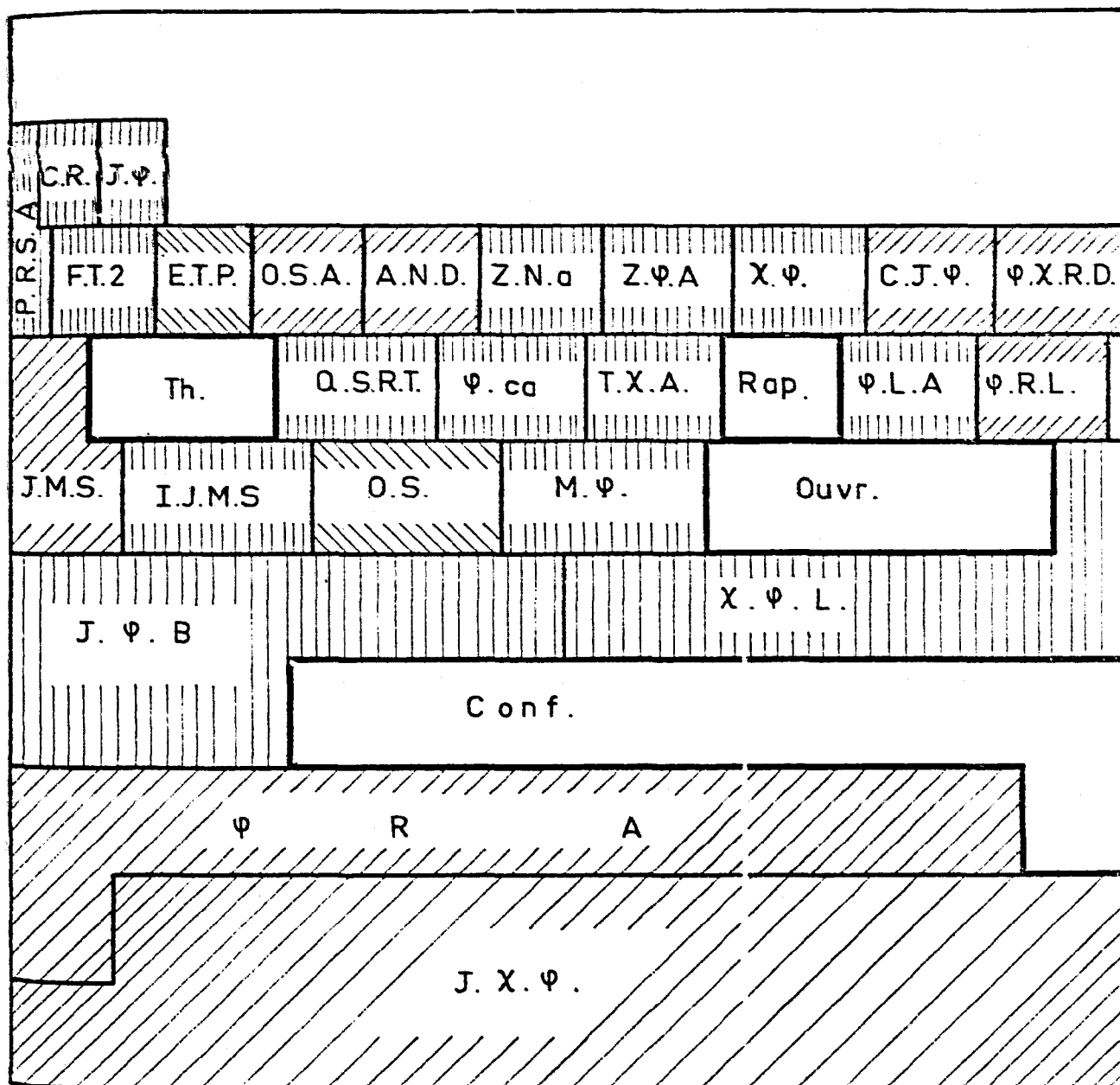


Fig. 3

scientific work of the various countries and their scientific publishing policies, geographical descriptors must be used, i.e. Country, Province or Town as they are defined in Ref. [2]. Unfortunately, we have but recently introduced these descriptors into GAPHYOR and we only have statistics on about 8000 lines (quarterly editions 1975 - 1 - 2 - and 3). With the necessary reservations about the imprecise nature of these statistics, we do, however, believe it useful to indicate the most striking findings.

Figures 4 and 5 show the relative importance of various countries as regards production (Fig. 4) or publication (Fig. 5) of GAPHYOR material. Table 4 shows the positions of the top nine countries from these two points of view.

It will be seen in particular that France's position as far as production is concerned (6.9 % of total production) is commendable, but is rather disastrous with regard to publications (0.8% of the total). It might be thought that this is due to the language problem; however, more detailed analysis will show that it is due more to a certain social and cultural behaviour of research people in France. In this connection we have characterized each of the nine most important countries with two indices:

The export index X_e of scientific work as defined by the formula:

$$X_e = \frac{\text{amount of GAPHYOR material published abroad}}{\text{total amount of GAPHYOR material produced in the country}}$$

and the import index X_i of scientific publications as defined by the formula:

$$X_i = \frac{\text{amount of foreign GAPHYOR material published in the country}}{\text{total amount of GAPHYOR material published in the country}}$$

The diagram of co-ordinates X_e and X_i in Fig. 6 shows how the different countries compare. The four sides of this diagram represent extreme behaviour:

- Nationalists $X_e = 0$ (no exports)
- Generous $X_e = 1$ (many exports)

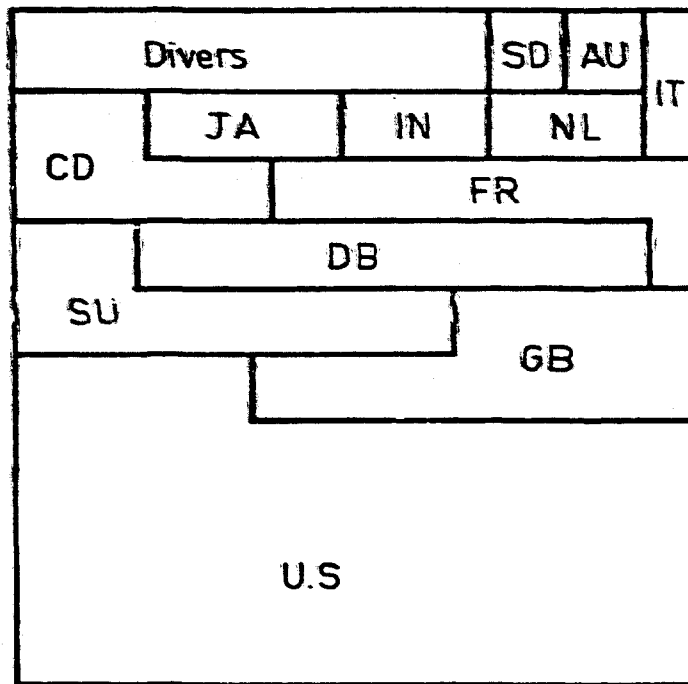


Fig. 4

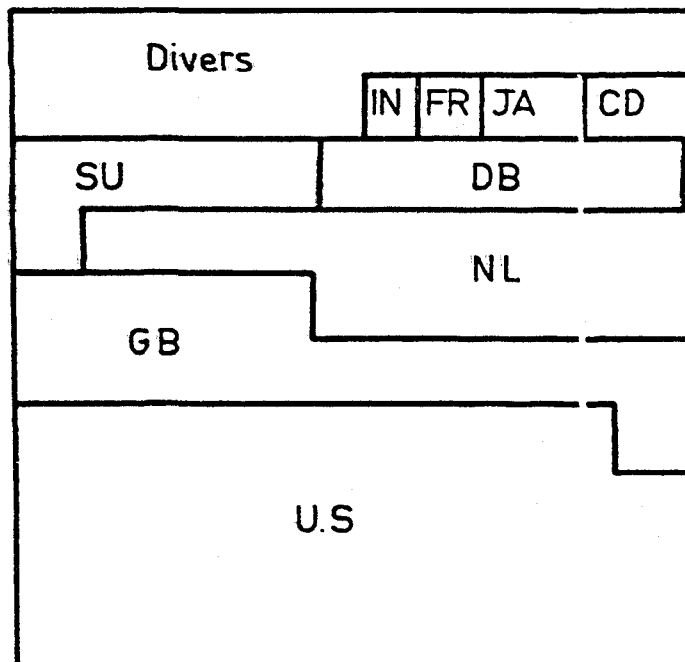


Fig. 5

TABLE 4 - Classification of countries according to production or publication of GAPHYOR material (the last column shows the difference between these two classifications)

| PRODUCTION | | PUBLICATION | |
|------------|-------------|-------------|---------------------|
| 1 | U S A | 1 | U S A (0) |
| 2 | U K | 2 | U K (0) |
| 3 | U R S S | 3 | N L (+ 6) |
| 4 | R F A | 4 | U R S S (- 1) |
| 5 | F R A N C E | 5 | R F A (- 1) |
| 6 | C D | 6 | C D (0) |
| 7 | J A | 7 | J A (0) |
| 8 | I N | 8 | F R A N C E (- 3) |
| 9 | N L | 9 | S U E D E (+ 3) |

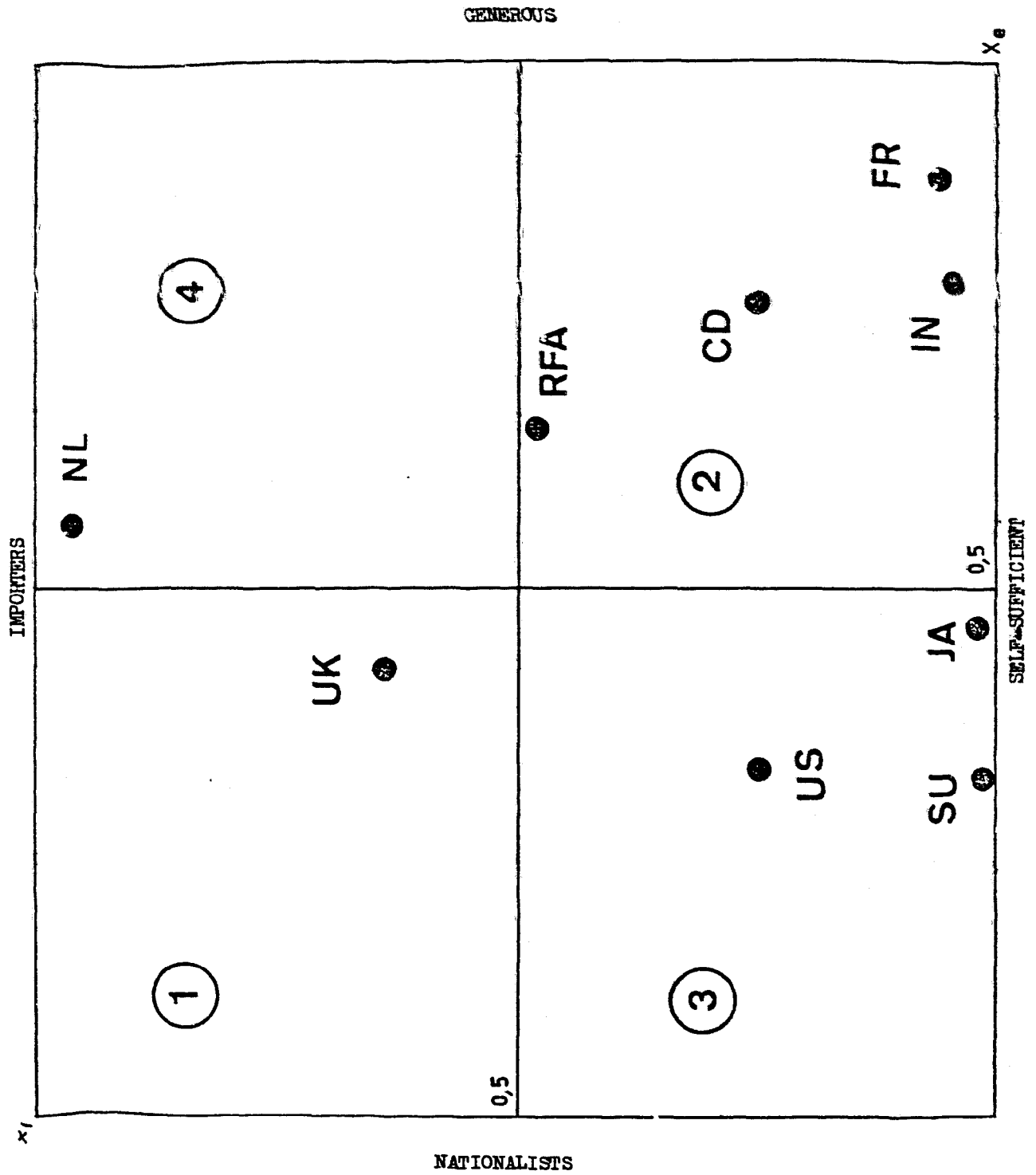


Fig. 6

- Self-sufficient $X_i = 0$ (no imports)
- Importers $X_i = 1$ (many imports).

It will be seen then that the first eight countries can be classified with regard to their scientific publishing policy in four groups:

Group 1 - nationalist and importer: United Kingdom, Netherlands;

Group 2 - generous and self-sufficient: France, Canada;

Group 3 - nationalist and self-sufficient: USA, USSR, Japan;

Group 4 - generous and importer: West Germany.

The countries in Group 1 publish the majority of their scientific results in their own country and succeed in attracting a large number of publications from other countries. These are the overall winners of Table 4.

The other countries in Group 2 only publish in their own journals a small proportion of their scientific results. Moreover, they succeed in attracting only very few publications from other countries. They are the overall losers of Table 4. France is the best example of this.

The countries in Groups 3 and 4 have an attitude which produces a certain equilibrium, as two opposing effects cancel each other out. They are either open in both directions (e.g. West Germany) or closed in both directions (e.g. USSR). The case of the USA is rather unusual in view of its dominant position in terms of production. Although it exports only a moderate amount in relative terms ($X_e = 0.27$), in absolute terms it is the leading exporter and its exports represent 29% of all material exported by all countries. It is also a significant importer in absolute terms (20% of all results exported go to the USA).

11.6.2. Statistics by towns in France

A more detailed analysis of the amounts of scientific material that various research centres produce can be made using the descriptor "Cité". The results of this statistical study are given for France in Fig. 7.

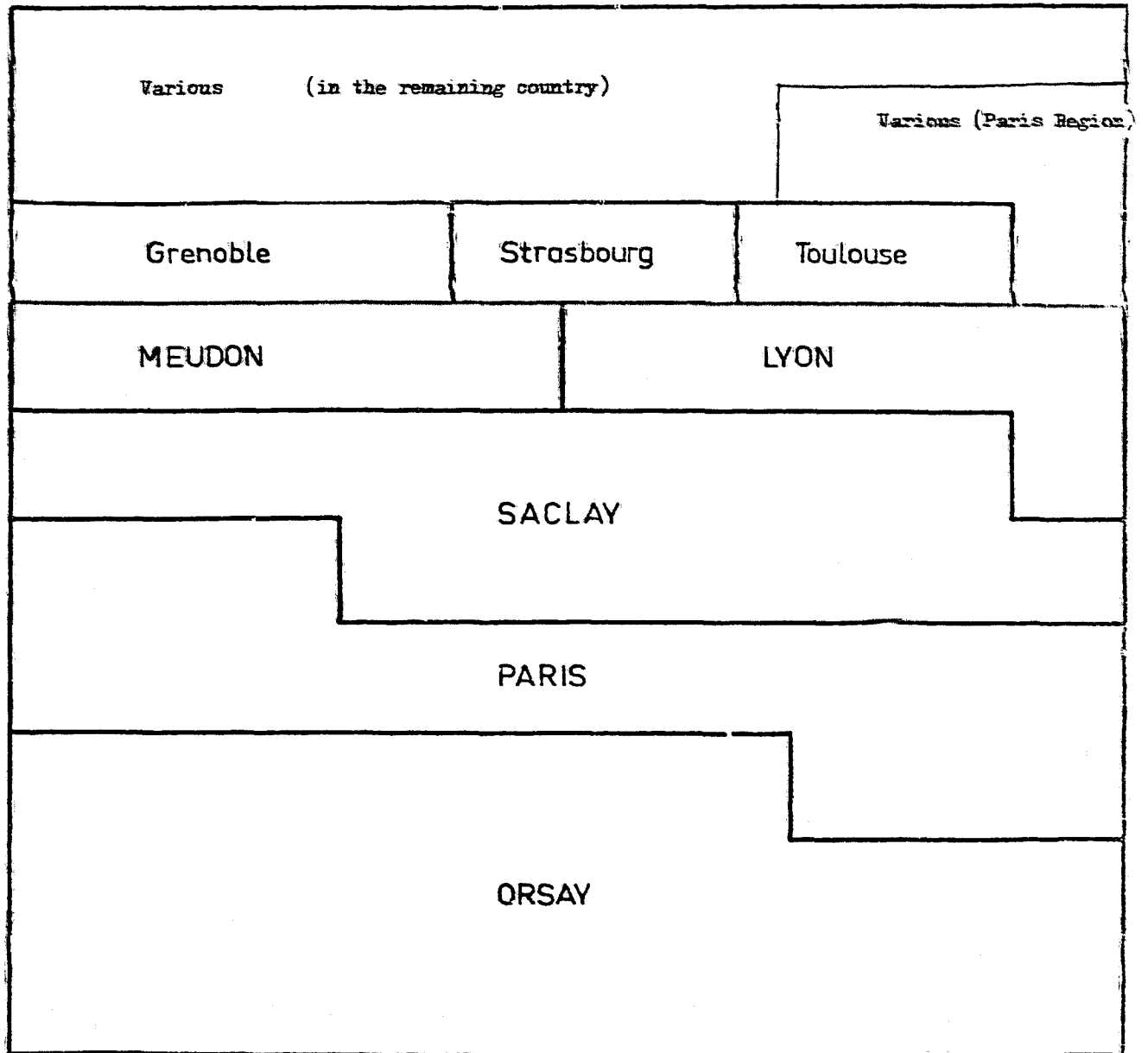


Fig. 7

12. CONCLUSION AND FORECASTS

12.1. Advantages of the GAPHYOR system

We believe that the GAPHYOR system offers a large number of advantages:

- it is not based on the use of more or less coordinated keywords, but on a quantitative code possessing internal logic and obeying syntax rules;
- the result is that Gaphyor allows a precise identification and arrangement of the data;
- in this manner it is possible to ask Gaphyor for information in various ways, according to the nature of the chemical system and the involved molecules on each reaction process, or other criteria (author, journal, ...); here, for instance, is one rather difficult problem which Gaphyor can solve immediately:
- to find and classify literature on the reactions which produce carbone monoxide.

12.2. Disadvantages of the GAPHYOR system and ways of improving it in the future

The advantages of the GAPHYOR system arise from the fact that its scope is strictly limited and that the relevant information lends itself quite well to a quantified logical description based essentially on conventional chemical notation, the Mendeleev periodic table and simple concepts of atomic and molecular physics. Nevertheless, there are two disadvantages in the present system which should be noted:

- (a) GAPHYOR clients consult our file by making a specific request each time they need it. This method of examination on request is the most flexible. Its main disadvantage is a certain slowness (3-5 days' wait, taking postal delays into account). Nor does it favour rapid expansion of our system. Consultation on request produces a sort of snowball effect, but it is a method that is slow in the beginning. For this reason we have for some time been proposing three consultation methods:

- Consultation on request
- Subscription to the whole file (4 instalments per year)
- Subscription to a specified part of the file (4 instalments per year).

It might be thought that in the long run the ideal method of consultation would be a conversational system allowing clients to consult our file directly by means of a visual display. In the present state of our experience this would seem dangerous to us, as it very often happens that we are asked to interpret questions put by clients so that the computer can provide them with the optimum response.

- (b) Also, it should be said that the operation of ambitious information systems like GAPHYOR raises certain manpower problems, since it presupposes the active participation of experienced research workers specializing in the field of interest. It is only in the last few months that we have been able to form a well equipped scanning team as a result of the participation of a number of laboratories.⁽¹⁾

-
- (1) As of Nov. 1, 1976, the Gaphyor team is composed of the following staff:

Scanning: J.L. Delcroix*, A. Ricard*, F. Lafont* (Orsay)
A.M. Diany*, M. Locqueneux* (Paris VI)
J.M. Baronnet, J. Rakowitz (Limoges)

Computer processing and Management:

C. Leprince, C. Helft, D. Lecroc, R. Briquin*,
E. Claudon*.

*) on part time basis.

BIBLIOGRAPHICAL REFERENCES

Internal reports

- [1] GAPHYOR code of journals. Plasma Physics Laboratory,
Université de Paris-Sud, Centre d'Orsay.
- [2] GAPHYOR geographical code. Plasma Physics Laboratory,
Université de Paris-Sud, Centre d'Orsay.
- [3] Special conventions associated with the GAPHYOR code. Plasma
Physics Laboratory, Université de Paris-Sud, Centre d'Orsay.
- [4] Rapport L.P. 156, p. 35 - 37 - Plasma-physics Laboratory,
Université de Paris-Sud, Centre d'Orsay (February 1976).

FIGURE CAPTION

Fig. 1 - Statistical analysis of data concerning the systems with 1, 2, 3, 4 or 5 elements.

Fig. 2 - Statistics concerning "Families" ($\Sigma = 22.000 - 1-8-75$)

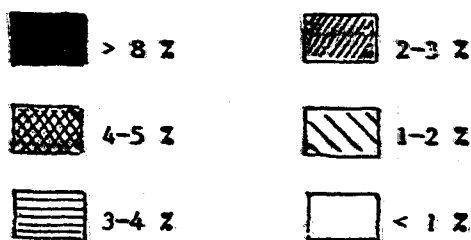


Fig. 3 - Statistics concerning "Journals" $\Sigma = 33.682$ (\int_0^{75-3})

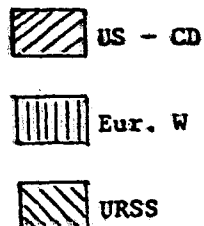


Fig. 4 - Production of "GAPHYOR" material (Jan. 1975 - Oct. 1975).

Fig. 5 - Publications of "GAPHYOR" results (Jan. 1975 - Oct. 1975).

Fig. 6 - Policies of various countries concerning scientific editing (for the definitions of x_e and x_i).

Fig. 7 - Production of "GAPHYOR" results concerning France (Jan. 1975 - Oct. 1975).

APPENDIX A

Dimensions of the GAPHYOR file

A1 Statement of the problem

The indexing descriptors of a computer card are:

- the Mendeleev families A, B, C, D;
- the process category K;
- the initial-state molecules P, Q, R;
- the simplified descriptor IS;
- the final-state molecules S, T, U; and
- the year and the file number.

Leaving aside the year and the file number, which complete the indexing operation, we shall consider that a compartment of the file is defined by a set of the descriptors ABCD, K, PQR, IS, STU. In this Appendix we propose to estimate the number of distinct compartments in GAPHYOR files 1, 2, 3 and 4.

A2 Number of ABCD family groups

The number of family groups is easily calculated as follows:

| | | | |
|-----------|--------------------|-------|-------|
| GAPHYOR 1 | groups of type A | | 24 |
| | | | — |
| GAPHYOR 2 | groups of type AB | 276 | |
| | groups of type AA | 24 | |
| | | | — |
| | Totals: | | 300 |
| GAPHYOR 3 | groups of type ABC | 2 024 | |
| | groups of type AAB | 276 | |
| | groups of type ABB | 276 | |
| | groups of type AAA | 24 | |
| | | | — |
| | Totals: | | 2 600 |

| | | |
|-----------|---------------------|--------|
| GAPHYOR 4 | groups of type ABCD | 10 626 |
| | groups of type AABC | 2 024 |
| | groups of type ABBC | 2 024 |
| | groups of type ABCC | 2 024 |
| | groups of type AABB | 276 |
| | groups of type AAAB | 276 |
| | groups of type ABBB | 276 |
| | groups of type AAAA | 24 |
| Total: | | 17 550 |

Obviously, these numbers are fairly high. To appreciate the simplification achieved through choosing the families A, B, C, D as indexing descriptors and not the elements 'XYZZ' themselves, one must compare these numbers with those which one would have with the elements:

| | | |
|-----------|--------------------|--------|
| GAPHYOR 1 | 97 | (4.04) |
| GAPHYOR 2 | 4 656 | (15.5) |
| GAPHYOR 3 | 1.47×10^5 | (56.5) |
| GAPHYOR 4 | 3.46×10^6 | (197) |

The figures in parentheses are the ratios of these numbers to the earlier ones.

A3 Number of molecules P

A molecule P is defined by:

- the indices $l m n p$, which define the general chemical formula; and
- the excitation and ionization indices $i x$.

The last two do not pose any problem; in general, they can assume ten values each and the number of possible combinations for $i x$ is 100.

The number of $l m n p$ formulas is rather more difficult to calculate as it is limited by the condition:

$$l + m + n + p \leq M = 8 \quad (1)$$

which we have imposed. Each of the indices $l m n p$ can assume a priori the $M + 1$ values $0, 1, 2, \dots, M$. If one takes the condition (1) into account, one can calculate the numbers of different $l m n p$ formulas P_1, P_2, P_3 and P_4 in GAPHYOR 1, 2, 3 and 4 respectively, obtaining:

| | |
|-----------|---|
| GAPHYOR 1 | $P_1(M) = M + 1$ |
| GAPHYOR 2 | $P_2(M) = 1 + 2 + \dots + (M+1) = (M+1)(M+2)/2$ |
| GAPHYOR 3 | $P_3(M) = P_2(0) + P_2(1) + \dots + P_2(M)$ |
| GAPHYOR 4 | $P_4(M) = P_3(0) + P_3(1) + \dots + P_3(M)$ |

Table A1 below gives the numerical values of these four numbers for values of M from 1 to 9.

We have ringed the results in the $M = 8$ column, which correspond to the choice made in the present version of GAPHYOR. With this table, therefore, one can estimate the extent of the simplification if one decided to confine oneself to a lower value of M .

A4 Dimensions of the "GAPHYOR" file

From the calculations performed in the two preceding sections it is possible to estimate approximately the number of compartments contained in GAPHYOR 1, 2, 3 and 4. The principle of the estimates is represented in Table A2. The total number N of compartments in the last line is obtained by multiplying the numbers of cases by each descriptor. It must be borne in mind, however, that not all the descriptors are independent variables:

- The volume of the file is determined essentially by $K = 4$ (collisions between heavy particles), or more precisely by the ternary collisions. The statistical weight of the descriptor K is therefore only 1. The same applies to the descriptor DS , for in the $K = 4$ category it is always associated with binary collision processes, the weight of which is negligible;

- The factors 1/6 introduced after PQR and STU take into account the fact that the orders of writing PQR and STU are imposed;
- The statistical weight of the molecule U is reduced to 10 since only its excitation index is an independent variable, its indices i m n and j being in general fixed (once PQEST are known) by the rules of conservation of the chemical elements and of electricity.

In brief, we find that the numbers of compartments of GAPHYOR files 1, 2, 3 and 4 are:

$$\begin{array}{ll} N_1 \sim 4 \times 10^{15} & N_3 \sim 10^{24} \\ N_2 \sim 1.5 \times 10^{20} & N_4 \sim 1.5 \times 10^{27} \end{array}$$

Hence, these are files whose theoretical volume is extremely large. In practice, only a very small fraction of this volume is "occupied" since at present we have only 33 000 cards. A very incomplete study of the file structure made in October 1976 (GAPHYOR 3 had been started only nine months previously) yielded the results presented in Table A3 as regards the number of family groups actually occupied. We shall try in future to analyse in greater detail the statistical structure of the known information and to introduce the concept of the "useful volume" of a file.

TABLE A1 - Numbers of $\ell m n p$ formulas with $\ell + m + n + p \leq M$

| M | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|-----------|---|---|----|----|----|-----|-----|-----|-----|-----|
| GAPHYOR 1 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| GAPHYOR 2 | 1 | 3 | 6 | 10 | 15 | 21 | 28 | 36 | 45 | 55 |
| GAPHYOR 3 | 1 | 4 | 10 | 20 | 35 | 56 | 84 | 120 | 165 | 220 |
| GAPHYOR 4 | 1 | 5 | 15 | 35 | 70 | 126 | 210 | 330 | 495 | 715 |

TABLE A3 - Number of occupied family groups (see text)

| GAPHYOR 1 | GAPHYOR 2 | GAPHYOR 3 |
|-----------|-----------|-----------|
| 24 | 133 | 85 |

TABLE A2 - Dimensions of GAPHYOR files 1,2,3 and 4

| Descrip- tors | GAPHYOR 1 | GAPHYOR 2 | GAPHYOR 3 | GAPHYOR 4 |
|------------------|-------------------|---------------------|------------------|---------------------|
| A | 24 | - | - | - |
| A B | - | 300 | - | - |
| A B C | - | - | 2600 | - |
| A B C D | - | - | - | 17550 |
| K | 1 | 1 | 1 | 1 |
| P | $9 \cdot 10^2$ | $45 \cdot 10^2$ | $165 \cdot 10^2$ | $495 \cdot 10^2$ |
| Q | $9 \cdot 10^2$ | $45 \cdot 10^2$ | $165 \cdot 10^2$ | $495 \cdot 10^2$ |
| R | $9 \cdot 10^2$ | $45 \cdot 10^2$ | $165 \cdot 10^2$ | $495 \cdot 10^2$ |
| X | 1/6 | 1/6 | 1/6 | 1/6 |
| D S | 1 | 1 | 1 | 1 |
| S | $9 \cdot 10^2$ | $45 \cdot 10^2$ | $165 \cdot 10^2$ | $495 \cdot 10^2$ |
| T | $9 \cdot 10^2$ | $45 \cdot 10^2$ | $165 \cdot 10^2$ | $495 \cdot 10^2$ |
| U | 10 | 10 | 10 | 10 |
| X | 1/6 | 1/6 | 1/6 | 1/6 |
| N | $4 \cdot 10^{15}$ | $1,5 \cdot 10^{20}$ | 10^{24} | $1,5 \cdot 10^{27}$ |

APPENDIX B
SIMPLIFIED DESCRIPTION OF PROCESSES

Category 1

EN Energy levels, wave function
CP Compton profiles
DP Dipole moments
NP Multipole moments
PE Electric polarization
VR Curves of potential, structure of molecules
TR Transition probabilities, lifetimes

Category 2

AN Absorption
EL Elastic collision
P2 2-photon interaction
P3 3-photon interaction
PN Multiphoton interaction
EE Production of electrons

Category 3

SN Total and transport cross-sections
EL Elastic collision
ER Line emission
EE Production of electrons
PP Production of positive charge

Category 4

SN Total and transport cross-sections
EL Elastic collisions
TE Excitation transfer
DX Quenching
10 Charge transfer 10 (fast particles)
20 Charge transfer 20 (fast particles)

LN LN charge transfer (fast particles)
MP MP charge transfer (target particles)
LP LN/NP charge transfer
ER Line emission
EE Production of electrons
PP Production of positive charge

Category 5

ZT Partition functions
CO Correlations
PV Compressibility, equation of state, vapour pressure
FT Thermodynamic functions
DN Scattering
VI Viscosity
CT Thermal conductivity
DT Thermal diffusion
DM Diffusion of metastables
RN Relaxation in neutral gases
ME Electronic mobility
DE Electron diffusion
FI First Townsend coefficient
AT Attachment
DT Detachment
PC Power exchanges by electron - neutral collision
MI Ionic mobility
DI Ion diffusion
DA Ambipolar diffusion
RC Recombination
PD After-glows