

## FRENCH ORGANIC NOMENCLATURE

BY NOEL LOZAC'H<sup>1</sup>

Faculte des Sciences de Caen, France

French Organic Chemists as a whole have always been convinced of the usefulness of systematic nomenclature. The rapid growth of organic chemistry after 1860 rendered necessary some international agreement in this field. At the occasion of the 1889 exhibition in Paris, a committee was created, and after forty-five preliminary meetings held in Paris, the Geneva Congress proposed international rules in 1892.

German and French Chemists have had a leading influence in the elaboration of Geneva nomenclature, which, as a consequence, received rather good acceptance in France, in Germany, and in the surrounding countries, except for the "oic acid" nomenclature, for linguistic reasons peculiar to German languages.

A very important character of Geneva Rules was that they intended to give one official name for any organic compound.

Unfortunately Geneva Rules were far from finished and their coverage of organic chemistry was utterly insufficient.

On the other hand, the first World War diminished the Germano-French influence in Chemistry to the benefit of English-speaking Countries. Chemical Abstracts was gaining in importance, and had to create, for its own purpose, a nomenclature which would cover the ever increasing field of Chemistry. However, the Beilstein Handbook obviously was obliged to maintain its editorial policy giving, whenever possible, preference to Geneva names.

It was in these circumstances that Liège Rules were prepared. They were not intended to give official names as Geneva Rules did. They only tried to give a practical nomenclature without interfering with the editorial policies of Beilstein and of Chemical Abstracts.

In some way, the Liège Rules recognize the fact that a lot of Geneva names had failed to gain general acceptance, either because they seemed too complicated or because chemists were not sufficiently conscious of the fact that a good nomenclature is worth some real efforts.

As a consequence, Liège Rules gave up what was the essential purpose of Geneva Nomenclature: the creation of a unique and unequivocal official name for every organic compound.

Some of the motives of this renunciation can be understood. The main reason was probably the idea that chemical names ought to be simple. Unfortunately simple names are the apanage of simple compounds, and with the

discovery of complicated compounds, we have to accept complicated names.

Very good features of Geneva nomenclature have been sacrificed to the desire of simplifying the names at any cost. One of these features was the maintenance of the same parent name for all the functional derivatives possessing the same carbon skeleton. The relentlessness with which this fundamental principle has been fought by people who had nothing to give in exchange is truly beyond belief. As a matter of consequence, most "nomenclature conscious" people in France considered Liège Rules with mixed feelings. They welcomed this effort toward a more extensive treatment of nomenclature problems, but felt quite uneasy when confronted with the price paid: the more or less tacit renunciation of important principles included into Geneva nomenclature. They thought it necessary to complement and sometimes to amend Liège Rules, as was done in the "Traité de Chimie Organique," published under the editorship of V. Grignard in 1935 and after.

After the second World War, the English-written chemical literature gained still more importance, with the result that the Chemical Abstracts approach in nomenclature gained a larger acceptance in France, where several laboratories switched from Zentralblatt to Chemical Abstracts for their general documentation.

At the time of the Zurich Congress (1955), rules were agreed upon which provide a good coverage of hydrocarbons and heterocycles, but the revision of the nomenclature of functions was still to come.

The "Comité National de la Chimie" considered that this situation could not continue without real damage for the French Chemical nomenclature. A comprehensive text was needed as a guide for Authors, and more specially for beginners whose nomenclature had a tendency to become a hodge-podge of Geneva, Chemical Abstracts, and very personal procedures. Accordingly, the Bulletin de la Société Chimique de France of January 1957 published a set of rules intended to give proper guidance to French Authors.

These rules received good acceptance in France, and the unavoidable criticism was limited to special points of minor importance. The most controversial question seemed to be

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whether one should say "ethanoïque" only or "acide ethanoïque" for acetic acid. The basis of the work was the rules adopted in Liège and afterwards by the International Union of Chemistry. Some of the initial Geneva rules, left unchanged in Liège, also found their place.

However, the International rules are, on some important points, very insufficient. Considering that Chemical Abstracts is the abstracting periodical most widely used by French Chemists, the French Nomenclature Committee thought it reasonable to follow their practice where International Rules are not sufficient and when there is no strong interference with established French habits. For instance, until an International rule is made, it has been decided to follow most of the Chemical Abstracts practices concerning the placing of prefixes and suffixes.

As they stand, the rules which have been published in the Bulletin de la Société Chimique are not stringent and leave the possibility of too many names. This was unavoidable. Otherwise there would have been a great risk of having these rules conflict with International rules now under consideration.

## NOMENCLATURE OF HYDROCARBONS AND HETEROCYCLES

Let us now turn to some specific problems which need consideration. The Paris Rules (1957) are the basis of French nomenclature for hydrocarbons and heterocycles. These rules reflect a great effort toward codification of existing practice. They have already received long discussions in order to find satisfactory compromises. However, general acceptance was not possible for every rule, and this situation has led in some cases to the existence of "alternate" rules. French Authors, being accustomed to the names used in Chemical Abstracts probably will choose the rules corresponding to Chemical Abstracts practice. However, this practice does not seem entirely satisfactory in some instances and further amendments would be appreciated.

### (a) Polyspiro alkanes

The Chemical Abstracts names apply only to linear polyspiro arrays. The existing system cannot be used with branched arrays. Only the lengths of the connecting chains are given in Chemical Abstracts names. These numbers can be correlated to a structural formula only if a supplementary assumption is made. Here it is admitted implicitly that any ring cannot contain more than two spiro-atoms.

It would be useful to reconsider "polyspiroalkanes" rules in order to bring them in better alignment with the "polycycloalkanes" rules.

This can be accomplished easily by denoting supplementary spirounions just as supplementary bridges in polycycloalkanes. It is quite simple to consider a spiro-atom as a special type of bridge-head where both ends of one bridge are fixed.

This is shown in Figure 1.

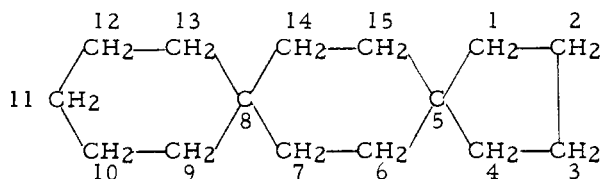


Fig. 1.1--C.A. numbering:  
Dispiro [4.2.5.2] pentadecane

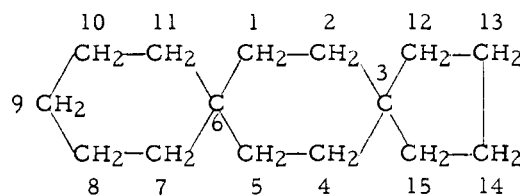


Fig. 1.2--Extension of v. Baeyer  
system: Dispiro [5.5.4<sup>3</sup>] pentadecane

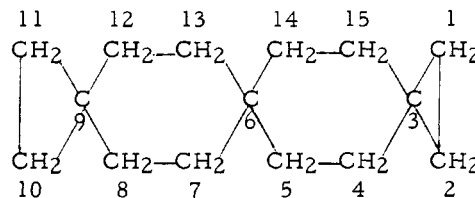


Fig. 1.3--C.A. numbering:  
Trispiro [2.2.2.2.2] pentadecane

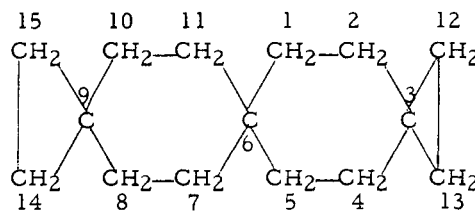


Fig. 1.4--Extension of v. Baeyer  
system: Trispiro [5.5.2<sup>3</sup>.2<sup>9</sup>] pentadecane

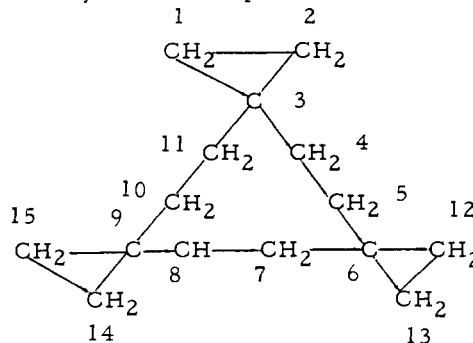


Fig. 1.5--Extension of v. Baeyer system:  
Trispiro [2.8.2<sup>6</sup>.2<sup>9</sup>] pentadecane

Figures 1.1 and 1.2 show in a simple case how the extension of the von Baeyer system can be made.

Figures 1.3 and 1.5 show what is meant by "implicit assumption" in the Chemical Abstracts system. If hydrocarbon 1.5 had to be named according to Chemical Abstracts methods, it could only receive the same name as 1.3. To the contrary, extended von Baeyer names, shown in 1.4 and 1.5 are specific.

On the other hand, spiro Chemical Abstracts names and von Baeyer polycyclic names cannot be combined, because the location of "supplementary" spiro unions is not directly given in spiro Chemical Abstract names.

On the contrary, the method we are considering can be extended easily to polycyclic structures containing fused rings and spiro unions, as shown in Figure 2.

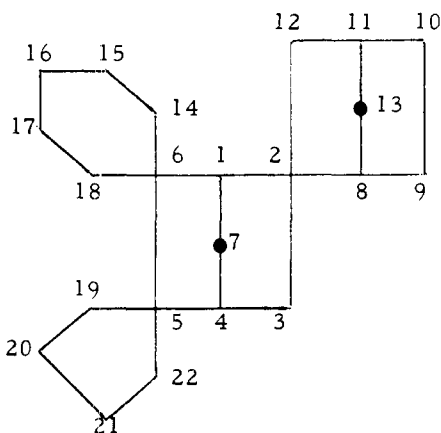


Fig. 2--Bicyclospirobicyclodispiro-[2.2.1.5<sup>2</sup>.1<sup>8</sup>,11<sup>5</sup>.6<sup>4</sup>.5<sup>1</sup>]docosane

#### (b) Numbering of fused heterocycles

Most French chemists consider that it is undesirable to give a different numbering to the skeleton when an heteroatom occurs in a fusion position. There is a tendency to maintain the numbering of the homocyclic analog. As the special numbering of fusion heteroatoms is used by Chemical Abstracts only in fusion names, the best solution is to use "a" names if it is desired to maintain the numbering of the homocyclic fused system.

The difference between the two methods is shown in Figure 3.

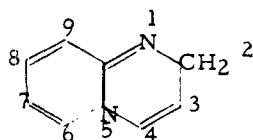


Fig. 3.1--C. A. fusion name:  
2H-Pyrido [1,2-a] pyrimidine

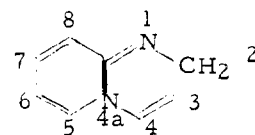


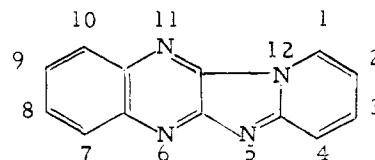
Fig. 3.2--Oxa-aza name:

2H-1,4a-Diazanaphthalene

Figure 3.1 gives the Chemical Abstracts name, and Figure 3.2 gives the oxa-aza name for the same compound.

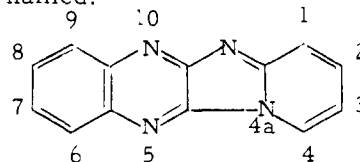
#### (c) Multiple fusion names

I refer to names such as:



Pyrido[1',2':1,2]imidazo[4,5-b]quinoxaline

This compound, with the oxa-aza convention, would be named:



4a,5,10,11-Tetrazabenzofluorene

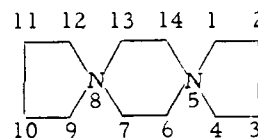
I expect that most French chemists will encounter great difficulties in coining multiple fusion names properly, that is to say, according to existing international rules. The oxa-aza method seems really simpler.

Multiple fusion names do not have the evocative power of simple fusion names, which give directly a general idea of the structure. It seems hopeless to use names implying three, four, etc., fusions.

A good solution would be a system such as that of Dyson-Taylor-Patterson.

#### (d) Poly-spiro-onium compounds

These compounds seem best named with "polyazonia" prefixes. For example:



5,8-Diazoniadispiro [4.2.4.2] tetradecane

Here also, the remarks previously made concerning the nomenclature of polyspiroalkanes should be taken into account.

## NOMENCLATURE OF FUNCTIONS

Chemical Abstracts has developed a method which is based mainly upon codification of current practice. The complexity of nomenclature is increasing each year, so a greater effort toward systematization is now necessary.

One can read in the Introduction to Liège Rules that official names are no longer necessary owing to the existence of formula indexes. Nevertheless, the number of entries under the same molecular formula can be so large that the usefulness of good official names is now evident. At least, a serious effort is needed in order to avoid an excessive proliferation of possible names for the same compound.

Existing practice evidently should receive proper consideration but, for further developments of nomenclature, it is extremely important to derive the rules from a limited number of clearly established principles.

I shall now consider how this rationalization of existing practice can be attained in some particular cases.

### (a) Skeletal nomenclature

According to this system, the skeleton of molecules is considered first. A parent compound is the one which contains the maximum number of noncumulative double bonds permitted by the skeleton. It happens that the name applies equally to isomers differing by the position of one or more hydrogen atoms in the structure. Then, the name can be made specific by indicating the position of such hydrogen atoms. For this purpose the name is preceded by the locant(s) of the hydrogen atom(s), followed by italic capital H for each atom.

In International rules, skeletal nomenclature is already described for hydrocarbons and fundamental heterocycles. The same method is also used by Chemical Abstracts for some functional derivatives, but with a special convention for indicated hydrogens, which appear between parentheses.

The trouble is that skeletal nomenclature has the same terminology as classical substitutive nomenclature.

Examples: Oxa-, Aza- prefixes,  
-one, -thione suffixes

Thus, it is important to make a clear cut distinction between the terms which are used with a skeletal meaning and those which are only used with a substitutive meaning. The usefulness of the idea of "main name" is that it sets a clear distinction between different parts of a complex name for which different logical methods are used. It would be the subject of a clear rule to say that the skeletal principle, with all its consequences concerning the state

of hydrogenation, should be applied to the "main name" considered as a unit. In fact, when this question was raised some years ago before the French Nomenclature Committee, we reached the conclusion that it was neither simple nor logical to treat indicated hydrogen in two different ways.

This point of view leads to names such as those given in Figures 4.1 and 4.2. Here, the keto group or groups are considered as part of the skeleton and indicated hydrogen is considered afterwards, only if necessary.

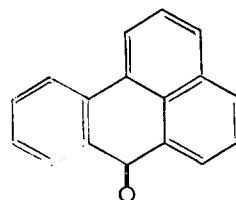


Fig. 4.1 -- Benz [d,e]anthracen-7-one

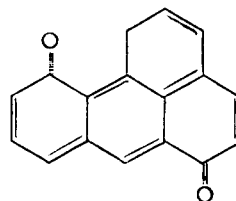


Fig. 4.2 -- 1H-Benz [d,e]anthracene-6, 11-dione

This point of view leads to a reappraisal of the status of hydro prefixes which is considered next.

### (b) Place of the "Hydro" prefixes

These prefixes are now mixed with the other prefixes denoting substitution. This is quite illogical and leads to trouble. It would be far better to admit that substitution prefixes apply to the "main name" considered as a whole.

The main name should contain the hydro prefixes, because hydrogenation of the structure often needs to be made before substitution is possible.

The case for hydro prefixes is the same as for "a" prefixes. Both types of prefixes may presume of substitution and should be included within the main name. The logical place for hydro prefixes is immediately before indicated hydrogen, because the chemical meaning of the hydro locants is strictly identical with the meaning of the indicated hydrogen locant. For instance, the 1,2-dihydro derivative of 3H-benz [d,e]anthracene is 2,3-dihydro-1H-benz [d,e]anthracene. This is the reason why French Rule F.4 (Bull. Soc. Chim. 1957, p. 59) proposed the following scheme:

## Substitution prefixes

Main name	Hydro prefixes
	Indicated hydrogen
	"Oxa-aza-etc.," prefixes
	Parent name, including fusion prefixes
	Unsaturation suffixes
	Functional suffixes

For indexes, such a main name would constitute a good main entry. For instance 1,2,3,4-tetrahydronaphthalene derivatives would occur under the same heading, which is much more satisfactory from the chemical point of view.

## (c) Choice of the principal function

For the time being, French Authors are requested to use the seniority order adopted in Liège. When the Liège Rule is not sufficient, the Chemical Abstracts names often are used as models for the choice of the principal functions. The task would be made much easier if a general seniority rule were available. Such a rule should codify existing practice and introduce as few changes as possible.

If this seniority order is to be used only for the choice of the "principal function," we do not have to consider functions which can be expressed only by prefixes, for instance:

F, Cl, Br, I, NO, NO<sub>2</sub>, PO, PO<sub>2</sub>, IO, IO<sub>2</sub>, ClO<sub>3</sub>

The "acinitro" group ( $\text{N} \begin{smallmatrix} \text{O} \\ \diagup \end{smallmatrix} \text{OH}$ ) should not belong to this group. It should receive the same treatment as phosphinic acids ( $\text{P} \begin{smallmatrix} \text{O} \\ \diagup \end{smallmatrix} \text{OH}$ ).

The choice of the principal function is the choice of the ending of a name, and the matter has been somewhat obscured by a long lasting confusion between ionic names and radico-functional names.

When a name is given to an ion, the ionic endings -ium, -ate, -ide ought to be used in most cases. A few exceptions seem useful, such as the "diazonia-dispiro" names.

For a salt, the names of two ions are given:

Examples: Tetramethylammonium benzoate  
1-Methylpyridinium 4-hydroxy-  
benzothiazolyl-2-sulfide

Radico-functional names, although designating non-ionic compounds, are somewhat similar to ionic names, the cation only being replaced by a radical.

Examples: Ethyl benzoate  
Butyl methyl sulfide

Ionic names are required for a correct description of the chemical structure. To the contrary most radico-functional names may be replaced by substitutive names.

In English names, the so-called "functional ending" is sometimes really a suffix, but it also may be the end of radico-functional name such as "pentanoyl chloride." In French "pentanoyl chloride" is translated by "chlorure de pentanoyle," and in French the equivalent of the so-called functional ending "oyl chloride" does not exist, because "Chlorure" ought to come at the beginning and not at the end of the name.

This difference should always be borne in mind when comparing French and English nomenclature for this type of name. It is not a question of chemical nomenclature but of grammar.

As a rule, this inversion of the name is to be found for oxyacids (carboxylic, sulfonic, etc.), their esters and their halides. The choice of such a function as the principal one means that the name should be of the substitutive-functional (e.g., acide benzene sulfonique) or of the radico-functional type (e.g., Chlorure de benzoyle).

In French, radico-functional names are less favored for ethers and sulfides, the prefixes "alkoxy," etc., "alkylthio," etc., being preferred, even if there is no other functional ending.

These habits are firmly rooted in the mind of French chemists and to advocate a drastic change has some chance of success only if we can offer a really better alternate system, with a convenient and clear seniority order of the functions. If such a system is proposed on an international basis, I am quite sure that French chemists will make an effort to get rid of old habits. On the contrary, one cannot hope to enforce a rule in France concerning principal functions without a good logical basis, which by the way, would be equally useful to non-French-speaking people.

This problem has so many implications that we can't discuss it here in detail. We wish only to say that it seems possible to generalize the seniority order used by Chemical Abstracts without resorting to drastic changes.

## (3) Conjunctive and Geneva names

Chemical Abstracts does not seem to like Geneva radical names with functional endings such as in "anthracene dipentylol" or "anthracene trimethylol." The principal advantage of these names is to preserve the functional ending. The same result has been obtained in Chemical Abstracts through the use of conjunctive names such as "anthracenedipentanoic acid" or "anthracenetrimethanol."

The use of the latter names is steadily increasing, and this shows the correctness of the Geneva proposals which gave a possible solution some 70 years ago. Some French authors still use the alkyloic names in conformity with Liege Rules, which maintain Geneva Rules for acids. There is a good reason for this: the French language is reluctant to use compound words.

In English, it is quite common to put two substantives side by side. In French some idea of subordination of one substantive to the other is needed. In the chemical field this idea of subordination is expressed by the "yl" particle. However, the difference between the two methods is not very important, provided that the numbering of the structure is always the same. If the side chains are always numbered in the same way, it does not matter very much whether "naphthalene butyloic acid" or "naphthalene butanoic acid" is written.

## CONCLUSION

Despite some differences, French and English nomenclatures in organic chemistry are

very similar. The necessary development of systematic nomenclature should tend to increase the scope of the rules by building them upon general principles quite independent of the grammatical customs of any national language. This is why substitutive names are of great value for International use.

And last, but not least, in a field where the grammatical habits do not interfere, special efforts ought to be exerted to achieve a generally agreed upon system of numbering complex structures. A large quantity of work and money is lost every year through misunderstanding of numbering. The French Commission for Organic Nomenclature thinks that proper consideration should be given to a systematic numbering of organic structures such as the one set forth by the International Commission for Codification and Ciphering. The Dyson-Taylor-Patterson system for polycyclic structures has been published already in the Bulletin de la Société Chimique (1957, p. 45).

It is not easy for nomenclature to keep pace with the ever increasing results in chemical research. Great care should be given to the general logic of the system, because the logic of today is the practicability of tomorrow.