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A NEW SEQUENTIAL ENUMERATION AND LINE FORMULA NOTATION SYSTEM FOR ORGANIC COMPOUNDS

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PREFACE

Two propositions lie at the heart of the system of enumeration and notation described in this paper, viz:

1. The distribution of hydrogen atoms in a saturated hydro carbon is unambiguous and can serve as a basis for an unambiguous enumeration pattern.
2. The nature and distribution of derived features can be accommodated in a logical manner whereby the enumeration pattern of any derivative is always congruent with that of the parent saturated hydrocarbon.

After a year and a half of constant confrontation with the agonizing complexities of hydrocarbon configurations, the above notions, first put to test in April 1960, have finally evolved into the system reported here, which represents yet another effort in the continuing struggle of organic chemists to systematize what Wohler (1835) once described as "a primeval tropical forest, full of the most remarkable things, a monstrous and boundless thicket, with no way to escape, into which one may well dread to enter."

I gratefully acknowledge the encouragement and constructive criticism of Harold Pfeffer and Herbert R. Koller, Senior Staff members of the Office of Research and Development (HAYSTAQ project) of the U. S. Patent Office, and with particular gratitude to Harold Pfeffer who monitored all stages of development of the system for general validity.

I further wish to thank Ellen Isaacs and Justin Walker (now Freshmen at the University of Chicago and Carnegie Tech., respectively) who, as summer (1961) employees of the U.S. Patent Office, learned and tested the system, made helpful suggestions, and completed a logical flow-chart[15] designed to receive any cipher of the reported notation as input and to generate therefrom a pictorial display of the structural formula on the face of a cathode ray tube.

Additionally, I extend my appreciation to other chemists of the U.S. Patent Office, viz: Ernestine Conner Bartlett, Yvonne M. Harris, and Dale Robertson Mahanand, of the HAYSTAQ project, and Lucille M. Miller of the DRAM project, who ciphered and deciphered a number of compounds and/or otherwise helped to evaluate the system.

Finally, I extend my deepest gratitude to all of those eminent chemists who have published notation systems over the past decade and a half. Without the availability of these publications, which so richly endow the art with insight into the complexities of organic molecules, the development and reporting of the present system would have been much longer delayed.

Comments and criticisms by fellow chemists are invited. Any suggestion for improving the system will be welcomed.

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Contents

INTRODUCTION

The system of notation for organic structures presently proposed represents an attempt to meet the desiderata laid down in 1949 by the Commission on Codification of the International Union of Pure and Applied Chemistry (IUPAC). The desiderata are as follows:

1. Simplicity of usage.
2. Ease of printing and typewriting.
3. Conciseness.
4. Recognizability.
5. The ability to generate a unique chemical nomenclature.
6. Compatibility with accepted practices of inorganic chemical notation.
7. Uniqueness.
8. Generation of an unambiguous and useful enumeration pattern.
9. Ease of manipulation by machine methods.
10. Exhibitions of associations (descriptiveness).
11. Ability to deal with partial indeterminants.

Since 1949 a number of notation systems, or ciphering schemes, have been in competition for international acceptance, particularly those separately proposed by Cockburn[1], Dyson[2], Gordon-Kendall-Davison[3], Gruber[4], Silk[5], and Wiswesser[6]. The Dyson system with modifications has been accepted as official by the IUPAC and is now published.[13] All of the schemes named above, and others, have been tested on organic compounds of varying degrees of complexity to illustrate the logical approaches of the several systems, and the results of such tests have been reviewed[8]. A survey of the development of chemical notation systems since 1946 (Dyson), including systems which are currently being explored by the Soviet Union, has recently (1961) been published[9].

Major features of the presently proposed system are described below in the context of their relationship to the above mentioned desiderata.

1. SIMPLICITY OF USAGE

A maximum of 64 different characters are used.

Atoms are ciphered, ignoring hydrogen attached to carbon, essentially on a one for one basis.

Each cipher is a valid line formula which can be deciphered without reference to an enumeration pattern.

The same basic rules for determining the order of enumeration and of ciphering apply to all organic compounds.

It seems to be generally characteristic of the present system to require a significantly smaller number of different characters per cipher (a measure of relative simplicity) than is required by the Dyson (IUPAC) notation system.

2. EASE OF PRINTING AND TYPEWRITING

All of the characters used are standard on typewriter keyboards, with the exception of delta "Δ" and braces "{ }". The latter may be substituted by (̶)̶, i.e., dashes superimposed upon parentheses, as suggested by Silk. The symbols assigned to the commonly occurring elements: C, O, N, S, P, and the halogens, except lower case "n" for ring nitrogen, are all capital letters. No subscripts or superscripts are employed.

3. CONCISENESS

Single bonds and hydrogen atoms attached to carbon are not ciphered but implied. The use of parentheses to set off substituents is minimized by assigning single character representations to the following high frequency groups:

B—for bromine
E—for ethyl (when not attached to "$-CH_2-$")
K—for chlorine
M—for methyl (when not included in T or attached to "$-CH_2-$")
Q—for hydroxy (OH)
T—for isopropyl
V—for oxo (=o)
W—for gem. dioxo (=o,=o)
Z—for primary amino (NH2)

The system does not give to conciseness as high a priority as to the preservation of the features exhibited by the structural formula being ciphered, since it is hoped that the cipher will be useful for information retrieval purposes by mechanical means.[7, 14] It is realized that the symbols E, Q, T, and Z do compromise the principle of a one to one relationship between atoms and their notation symbols. It may be more practical in cases where the system is engineered for automatic retrieval of information of highly refined degrees of specificity to represent E by (CM); Q, by (OH); T by (CM2); and Z, by (NH2).

Comparative studies on a small scale indicate that the present system compares favorably with the Dyson (IUPAC, 1958)* system in regard to both the total number of characters and the number of different characters which are required per given cipher, as indicated by the data below. The data is based on compounds which appear in the 1958 IUPAC notation system[10] and on ring aggregates which are included in the IUPAC test list of 100 special compounds.[8] The "D" columns relates to the Dyson system; the "H" columns to the present system.

4. RECOGNIZABILITY

Since no linear array of characters can do more than "code", or suggest, the geometric relationships which are generally characteristic of the classical two dimensional structural formula, it appears obvious that any linear cipher must suffer, in terms of recognizability, due to the loss of the vertical dimension. It is believed that line formula notation inherently has greater recognizability than "locant" notation, which identifies the locations of atoms by number, since the former exhibits the atoms in their configurational environment without the interruption of "locants" which, by themselves, have no chemical meaning.

5. ABILITY TO GENERATE A UNIQUE CHEMICAL NOMENCLATURE

A fundamentally sound basis for establishing a unique nomenclature for organic compounds would appear to be inherent in any system which generates an unambiguous enumeration pattern which assigns a unique number to each skeletal atom. An obvious procedure consonant with the present system would be to name, first, in a systematic way, all classes of saturated hydrocarbons. It would then be possible to reference derived features by stating their numerical position, or "address", in the enumeration pattern.

6. COMPATIBILITY WITH ACCEPTED PRACTICES OF INORGANIC CHEMICAL NOTATION

Application of the system to inorganic compounds is beyond the scope of this paper. It may be worth mentioning, however, that any inorganic ring, of which the atoms are necessarily covalently bonded, may be delineated as a derived hydrocarbon ring.

Inorganic ions of organic salts are ciphered by selecting as starting atom that atom of the ion which has the following properties in the order of decreasing priority:

(1) highest valence state, or
(2) heaviest atomic weight,

COMPOUND TYPE	NUMBER OF CPDS CIPHERED	AVERAGE # CHAR.		AVERAGE # DIF. CHAR.	
		D	H	D	H
Acyclic hydrocarbons saturated	7	15	12	9	6
Acyclic hydrocarbons Unsaturated	2	26	18	12	8
Acyclic hydrocarbon derivatives	34	21	13	11	7
Fused ring aggregates	27	37	16	28	9
Complex ring-chain assemblies	5	95	99	22	22
OVERALL	75	39	32	16	10

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*The official IUPAC notation system was not published at the time the studies were made.

then ciphering the remaining atoms in the order of their increasing atomic weights, using appropriate numerical suffixes where necessary to denote a plurality of a given atom.

7. UNIQUENESS

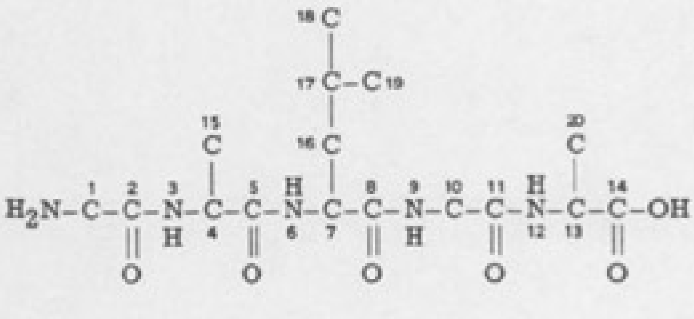
There is only one correct enumeration pattern for each molecule and only one correct cipher. Every molecule is ciphered as a static structure so that whatever structure is ciphered may be reconstituted by deciphering. Delineation of conformation features and of electron structures is beyond the scope of the cipher as presently described.

8. GENERATION OF AN UNAMBIGUOUS AND USEFUL ENUMERATION PATTERN

The enumeration of every saturated hydrocarbon is sequential and is based directly on the distribution of hydrogen atoms upon the carbon framework.

The enumeration pattern of each saturated hydrocarbon holds for all of its derivatives by accomodating derived features in a logical and unambiguous manner.

Since each skeletal atom - atom which corresponds to a carbon atom of the saturated parent hydrocarbon - is assigned a unique number, compounds can be indexed in an enumerative and hierarchical way, as illustrated below (or more concisely by using notation symbols):



Tetradecane; methyl-4, 13, 17; propyl-7.
aza-3, 6, 9, 12.
amino-1; oxo-2, 5, 8, 11, 14; oxy-14.

By "ciphering" the above name index (See cipher below) greater conciseness is achieved.

"Ciphered" Index (functional substituents arranged in order of increasing weight):

C14; M-4, 13, 17; C3-7. N-3, 6, 9, 12.
H-3, 6, 9, 12; V-2, 5, 8, 11, 14; Z-1; Q-14.

The enumeration pattern, in addition, serves to indicate in a simple way the order in which the atoms are ciphered.

9. EASE OF MANIPULATION BY MACHINE METHODS

A maximum of 64 different characters (no subscripts or superscripts used) are employed so as to permit their direct conversion by 6 binary bit coding (standard) into conventional machine language. A number of the 64 characters are reserved for assignment exclusively to "housekeeping" duties in stored logic devices, e.g., electronic digital computers.

10. EXHIBITION OF ASSOCIATIONS (DESCRIPTIVENESS)

The following symbols represent all atoms of the indicated element without reservation:

Symbol	For
B	bromine
F	fluorine
I	iodine
K	chlorine
P	phosphorus
S	sulfur

The following symbols represent the atoms indicated in their configurational environment:

Symbol	For
C	Carbon of open chain and of connecting link of a circular assembly.
L	Carbon of "L" type ring (special definition).*
N	Chain interrupting nitrogen.
n	Ring nitrogen.
O	Chain or ring interrupting oxygen.
Q	OH (hydroxy).
R	Carbon of "R" type ring (special definition).*
T	Isopropyl.
V	=o (oxo)
W	=o,=o, (gem. dioxo.)
X	spiro carbon
Y	ortho-fused carbon (peripheral)
y	peri-fused carbon (interior)
Z	NH_2 (primary amino)

The complete absence of "locants" from the cipher and the restriction on the multiplication of repeating chain and/or ring units to three or more, attached only to carbon, prevent the cipher from becoming "number-bound" and so lend the cipher a "molecular character" in the sense that the observing chemist is likely to feel that he is looking at atoms rather than at numbers.

The unfamiliarly assigned symbols B, E, K, M, n. T, V, W, X, Y, and y are believed to have mnemonic value in terms of the atoms they represent.

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*See Section 1.9.

11. ABILITY TO DEAL WITH PARTIAL INDETERMINANTS

The question mark "?" is used to denote indefinite number or position.

Three capital letters D, J, and U (as lone symbols), are reserved for dealing with partial indeterminants as are the tentatively allocated symbols (or others): "!, $, ¢".

Although each of the desiderata listed above makes compelling demands on any chemical notation system, a serious attempt has been made in the present system not to subserve any of the desiderata at the expense of failing to fulfill the ultimate aim of this notation, which is to establish a basis for a one to one relationship between (1) structure, (2) cipher, and (3) nomenclature, whereby any one of the three may be reconstructed from any one of the remaining two, and, hopefully, by datamatic processes.

Overiding all of the desiderata discussed above is the unifying philosophy of the present system, namely, that each organic molecule possesses a single continuous skeleton which may exist in either a virgin state-saturated hydrocarbon-or in a derived state-hydrocarbon derivative-and that the two states are interconvertible by a logical process while under the constraint, at all stages of interconversion, of an unambiguous and rigid enumeration pattern. It is hoped that the system will be useful for simplifying the problems of classifying, indexing, and naming organic molecules, and for representing them in a manner which will be independent of natural language. It is painfully recognized that any virile assault on the stated problems flirts with error and is seduced by pitfall; yet the struggle is continuous and is one for which the present system, as others before and now, must also gird itself. . .and join.

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1.0 CLASSIFICATION OF ORGANIC MOLECULES AND THEIR STRUCTURAL FEATURES. PARENT-SUBSTITUENT RELATIONSHIPS

In the present system each organic molecule is considered to have a single continuous skeleton which can be reduced to a corresponding saturated parent hydrocarbon by executing the following operations:

(1) stripping the molecule free of all atoms except carbon atoms, ring atoms, and hetero atoms which interrupt a carbon chain,

(2) replacing all hetero atoms of the structure residual to operation (1) by carbon atoms on a one for one basis, and

(3) saturating all multiple bonds and dangling valences of the structure residual to operations (1) and (2) by hydrogen atoms (implied).

1.1 CLASSIFICATION OF SATURATED HYDROCARBONS

The classification of an organic molecule, in the present system, gives highest priority to the structure of the corresponding saturated hydrocarbon - arrived at by the execution of operations (1) to (3), above, to the extent necessary - and is based first of all upon the ring structure, if any, of such hydrocarbon.

Saturated hydrocarbons are classified into the following groups listed in their order of increasing complexity:

I. Acyclics
II. Monocyclics
III. Fused Ring Aggregates
IV. Bridged Ring Aggregates
V. Ring Assemblies
  1. random
  2. circular

The enumeration and ciphering of each of the above classes I to V will be described in detail in Sections 3-7 of this paper in the order listed.

Molecules which are polymeric in nature are classified in group I or group V depending upon the structure of the repeating unit, and are discussed in Section 9.

1.2 CLASSIFICATION OF DERIVED FEATURES

A saturated hydrocarbon may be derived, chemically, only by one or more of the following three ways (excluding stereoisomeric relationships) without rupturing or enlarging the skeleton:

(1) by replacement of non-terminal carbon atoms by hetero atoms on a one for one basis,

(2) by replacement of individual hydrogen atoms by a hetero atom or acyclic group of hetero atoms, or

(3) by removal of pairs of hydrogen atoms to form multiple bonds between skeletal atoms.

Replacement of terminal carbon atoms, isomerization of the carbon skeleton, or replacement of a plurality of hydrogen atoms by the same polycovalent radical is forbidden since in each case a different parent hydrocarbon would be created. An ionic charge placed on an organic species is not considered to be a structurally derived feature of a parent carbon skeleton but rather an attribute of the species as a whole.

Related to their method of formation, as described above, derived features are classified into the following three types in the order of decreasing priority for purposes of enumeration:

(1) skeletal hetero atoms;
(2) functional substitutents;
(3) skeletal bonds.

Classification of derived features in the above manner makes possible the assignment of an unambiguous order of enumeration to skeletal paths which though symmetrical with respect to one another in the parent hydrocarbon are made unsymmetrical by some derived feature.

The classification of salts is based on the skeletal configuration of the organic ions involved. A salt may be classified into any one, or a plurality, of groups I-V above but primarily is classified in the group which bears the higher Roman numeral.

In the system of priorities which controls the order of enumeration - and presumably, by analogy, would hold for purposes of indexing and nomenclature - a skeletal hetero atom, type (1), a functional substitutent, type (2), or a skeletal bond, type (3), is superior to another of the same type which has the following features listed in their order of decreasing priority:

1. lower assigned number (skeletal position);
2. greater weight, or degree of unsaturation of bond.

The total classification of an organic molecule, as described above, preceded by gross indexing features, such as the

1. total number of skeletal atoms, and
2. number of skeletal atoms in the main chain or in the generating ring system

in the order listed, allows each molecule to be described from the broadest possible down to the narrowest possible structural feature and through all logical intermediate stages, within the limits set forth (See Introduction - UNIQUENESS). The system, in addition, is inherently open-ended in the sense that no priorities need be changed in order to admit novel members to the organization.

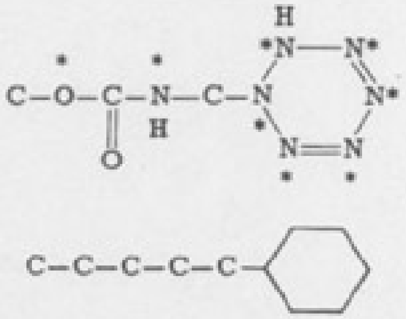
It is believed that the above classification principles are susceptible to suggested automation techniques for screening large scale files.[12]

1.3 DEFINITION OF SKELETAL ATOM AND SKELETAL BOND

A skeletal atom is a carbon atom or a hetero atom which corresponds to a carbon atom of the parent hydrocarbon.

In the following formula skeletal hetero atoms are labelled by asterisks. The parent hydrocarbon appears below the derived formula.

EXAMPLE:

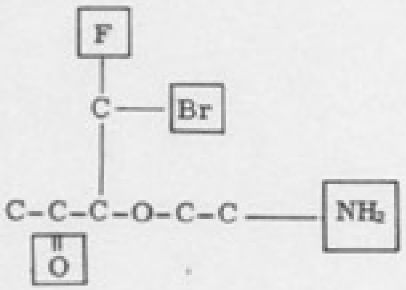


A skeletal bond is simply a bond which connects two skeletal atoms. In the described system a triple bond is more unsaturated than a double bond; any bond of an "R" ring, more unsaturated than a double bond of an "L" ring or open chain.

1.4 DEFINITION OF FUNCTIONAL SUBSTITUENT

A functional substituent is a terminal group of hetero atoms, or a terminal group constituted by a single hetero atom, which group contains no atom which corresponds to a carbon atom of the related parent hydrocarbon.

EXAMPLE:



The groups enclosed by rectangles are functional substitutents.

1.5 DEFINITION OF SKELETAL SUBSTITUENT

The definition is based upon the fully enumerated structural formula, enumerated according to the procedure described herein.

Whenever the lowest numbered atom of a group, or path, breaks the ascending numerical sequence of the lowest numbered atom to which such group is directly bonded then the group is a skeletal substituent of the latter lowest numbered atom, called the parent atom.

A group, or path, as described above, may be constituted by a single enumerated atom and its connecting bond.

1.6 TYPES OF SKELETAL SUBSTITUENTS

Skeletal substituents are classified into the following three types:

(1) acyclic;
(2) cyclic, or ring containing;
(3) bridge.

A substitutent of type (1) or (2) is always attached to its parent atom by an acyclic bond; a substitutent of type (3), by a ring bond.

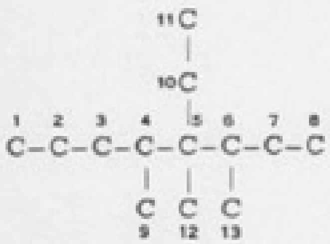
An acyclic skeletal substituent is one which contains at least one carbon atom but no rings.

A cyclic substituent is one which contains at least one ring.

A bridge substituent is one which consists entirely of ring atoms of the same discrete ring system to which its parent atom belongs. A ring bridge bears a substituent relationship to a particular atom of its related parent ring system, as will be explained and illustrated in section 6.2.

In the following examples the tabulated data appearing beneath each formula lists the identifying numbers of the parent atoms in the left column and the defining atoms of their corresponding substitutents in the right column:

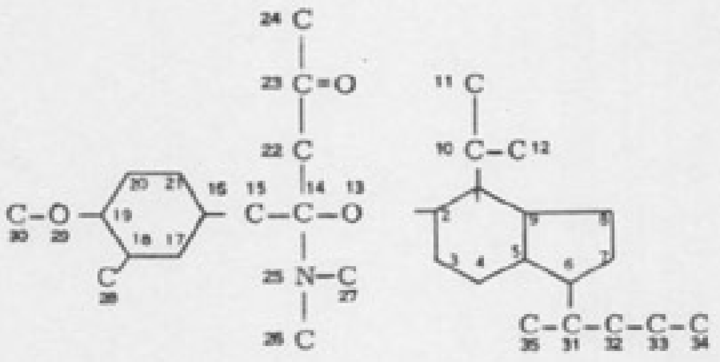
EXAMPLE:



Parent atoms	Substituent atoms
4	9
5	10-11
5	12
6	13

The substituents identified in the right column are all acyclic skeletal substitutents.

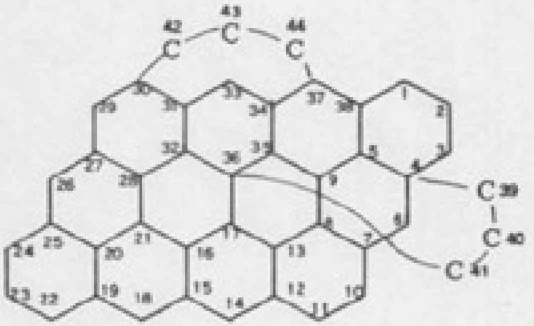
EXAMPLE:



Parent atoms	Substituent atoms
1	10-12
2	13-30
6	31-35
10	12
14	22-24
14	25-27
18	28
19	29-30
25	27
31	35

In the above formula the substituents of parent atoms "1, 6, 10, 14, 18, 19, 25, and 31" are acyclic skeletal substituents; the substituent of atom "2", a cyclic substituent, which includes acyclic substituents, as indicated above.

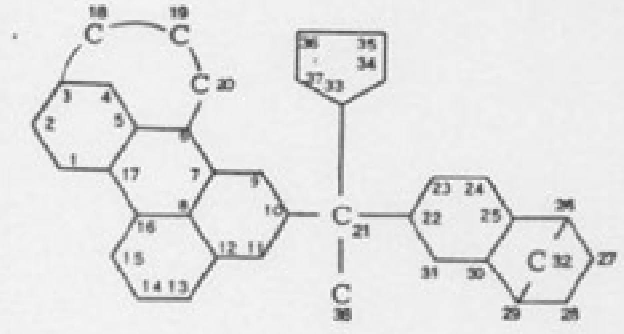
EXAMPLE:



Parent atoms	Substituent atoms
4	39-41
30	42-44

Atoms "39-41" and "42-44" are classified as ring bridges and are bridge substituents, of atoms 4 and 30, respectively.

EXAMPLE:



Parent atoms	Substituent atoms
3	18-20
10	21-38
21	33-37
21	38
26	32

Atoms "18-20" and "32", respectively, are bridge substituents of atoms "3" and "26", respectively; atoms "21-38", a single cyclic substituent of atom "10"; atoms "33-37", a cyclic substituent of atom "21"; and atom "38", an acyclic substituent of atom "21".

1.7 SUBSTITUENT CONTENT. DEFINITION.

The content of an acyclic or cyclic substituent consists of the bond by which it is connected to its parent atom and all atoms and bonds which are included in the group which is attached to said parent atom by such connecting bond.

A cyclic substituent includes all acyclic substituents and functional substituents included within its content, as defined above.

An acyclic carbon-containing substituent includes all functional substituents included within its content, as defined above.

1.8 SUBSTITUENT BOUNDARY SYMBOLS. PARENTHESES.

In any cipher which will not be used for automatic information retrieval purposes the boundaries of all substituents are denoted by enclosing the cipher of each substituent by parentheses.

If a compound cipher is intended to be stored on a medium which permits interrogation of the cipher mechanically for some part, as well as the whole, of its information content, then the boundaries of the three types of substituents, as defined above, may be indicated by three different sets of symbols-selected from those reserved-so that any substituent of a given type may be queried or ignored by stored logic techniques. In all ciphers presented in this paper parentheses are used to define substituent boundaries.

1.9 DEFINITION OF RING TYPES. "R" RINGS. "L" RINGS.

All rings except the connecting path of a circular assembly (see section 7.61), are classified into two groups: "R" rings and "L" rings.

An "R" ring is:

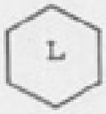
(1) any six-membered ring each atom of which is connected to one and only one ring double bond, or

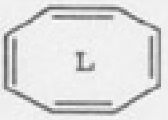
(2) any other ring each atom of which is connected to one and only one ring double bond provided that such ring is ortho-fused to a similarly bonded ring.

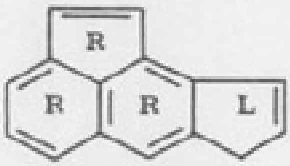
All rings which are not "R" rings as defined above, or fit the exception indicated, are classified as "L" rings.

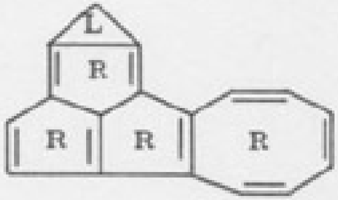
In the following examples all "R" rings are labelled by the symbol R; all "L" rings, by the symbol L:

EXAMPLES:









2.0 NOTATION SYMBOLS. GENERAL ENUMERATION AND CIPHERING PROCEDURE

2.1 ORDER AND METHOD OF PRESENTATION OF NOTATION SYMBOLS AND CIPHERS

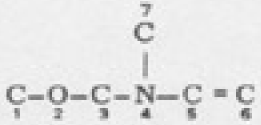
In order to save space all of the 64 symbols employed are presented in table form together with the specific rules which govern their use. The tables are placed at the end of the present section and are generally arranged so as to present the symbols which are more commonly used first. The final two tables are summary in nature and list the symbols and their principal use together with cross-referencing to pertinent information in other tables. Ciphers of representative compounds which illustrate the use of a given symbol are indicated by listing the identifying numbers-corresponding to numbers in the body of the text-of such compounds in the right-most column of tables XII and XIII.

The row of symbols beneath a given structural formula is the cipher of such formula. Any arabic numerals which appear from time to time above one or more of the symbols of a given cipher are not part of the cipher but serve to relate the symbol concerned to the atom which it represents. The enumeration and ciphering of saturated hydrocarbons and derivatives thereof will be discussed in the ascending numerical order of the group classifications I to V described in Section 1.1.

2.2 DEFINITION OF ENUMERATION PATTERN

The term "enumeration pattern" describes the fixed pattern of numbers which is assigned to the skeletal atoms of a structural formula in order to identify the relative positions of such atoms with respect to one another. Only skeletal atoms are enumerated.

EXAMPLE:



$$\underset{1}{C}-\underset{2}{O}-\underset{3}{C}-\underset{4}{\overset{\overset{\overset{7}{C}}{|}}{N}}-\underset{5}{C}=\underset{6}{C}$$

2.3 LOGICAL BASIS OF ENUMERATION

All atoms of a molecule which correspond to a carbon atom of the related saturated parent hydrocarbon are enumerated in ascending numerical order beginning with the number "1". The enumeration of each compound formula begins with that particular skeletal atom of such formula which generates the enumeration pattern which assigns the lower number to certain structural features in an order of decreasing priority. The order prescribed serves to establish an unambiguous enumeration pattern on the basis of what is considered to be the most constant and reliable feature of a given molecule.

The structural features which determine the origin and direction of the enumeration are listed below in their order of decreasing priority:

1. Configuration of the saturated parent hydrocarbon (virgin state)
2. weight and distribution of
    a. hetero atoms which interrupt a carbon chain or ring;
    b. functional substituents;
3. degree of unsaturation of skeletal bonds;
4. distribution of stereoisomeric features.

The system relies fundamentally upon the unambiguous distribution of hydrogen atoms in the saturated hydrocarbon state of organic molecules for the purpose of selecting for a given molecule an unambiguous:

(1) starting atom for the enumeration,

(2) direction of enumeration around a ring system, and

(3) order of enumeration of branches of an open chain.

In the enumeration of branches of an open chain in the virgin state the ascending enumeration always pursues that branching direction which is richer in carbon (most atoms) regardless of configuration, and when facing a tie on the basis of carbon content pursues that direction which becomes first richer in hydrogen, i.e. generates the ascending enumeration pattern which assigns the lower number on the occasion of the first difference-while obedient to the order of ascending enumeration prescribed hereafter for the particular type of path concerned—to that carbon atom which bears the greater number of hydrogen atoms.

The same principle applies to the order of enumeration of a plurality of skeletal substituents bonded to the same ring atom and to the direction (clockwise or counter-clockwise) of enumeration around a component ring system of a ring assembly after the enumeration of the first atom thereof.

2.4 GENERAL ORDER OF ASCENDING ENUMERATION OF SKELETAL PATHS OF ORGANIC MOLECULES

The skeletal paths of organic molecules are enumerated in the ascending numerical order in which they are listed below under the particular class to which a given molecule belongs:

- I. Acyclic:
    1. Main chain from one terminal carbon to another;
    2. Skeletal substituents (side chains), if any, in the ascending numerical order of the main chain atoms to which bonded;
- II. Monocyclic:
    1. Ring atoms, serially around the ring;

2. Skeletal substituents, if any, of ring in the ascending numerical order of the ring atoms to which bonded;

III. Fused ring aggregate:
   1. Ring system atoms, sequentially in the manner described in Sec. 5.;
   2. Skeletal substituents, if any, in the ascending numerical order of the ring system atoms to which bonded;

IV. Bridged ring aggregate:
   1. Atoms of planar parent ring system in the manner described for the class (II or III above) to which the planar system belongs;
   2. bridge(s), in the ascending numerical order of the lowest numbered parent planar ring atoms to which bonded as described in Sec. 6.;
   3. Skeletal substituents, if any, of bridged ring system, in the ascending numerical order of the ring system (bridge(s) included) atoms to which bonded;

V. Ring assembly (random or circular):
   1. generating ring system (Sec. 7.) according to the class (II, III, or IV) to which it belongs.
   2. skeletal substituents of the generating ring systems, in the ascending numerical order of the generating system atoms to which bonded.

It is a declared law of the system that once the enumeration of a planar ring system, bridge, or skeletal substituent has begun, in the order described above, the enumeration must proceed to the exhaustion of all skeletal atoms thereof before proceeding to the next skeletal path in order.

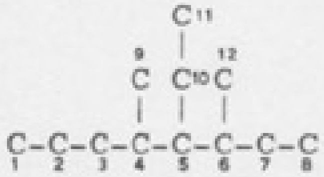
The specific order in which the atoms which constitute each of the several types of skeletal paths are enumerated and the criteria for selection of a starting atom for the enumeration of a molecule of a given class are set forth in the appropriate one of sections 3-7.

2.5 MOLECULES HAVING NO SYMMETRICAL PATHS IN THE SATURATED HYDROCARBON STATE

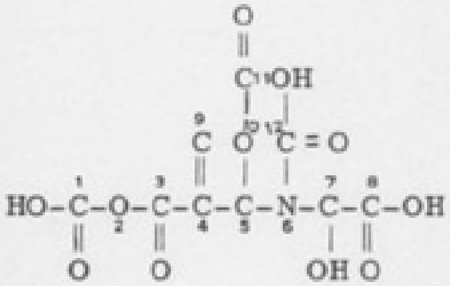
The enumeration pattern of an organic molecule whose virgin (saturated hydrocarbon) state contains no carbon paths which are symmetrical with respect to a point (skeletal atom or bond) in such molecule is unique and serves directly for any derived state without regard to the nature or distribution of derived features.

EXAMPLES:

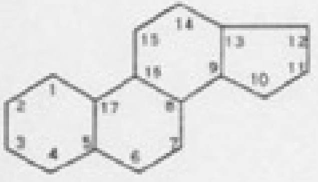
(1)



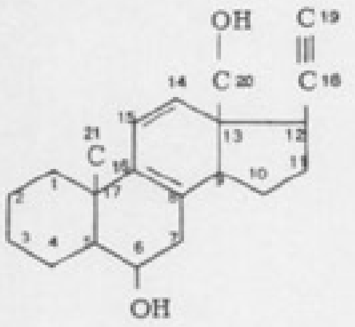
(2)



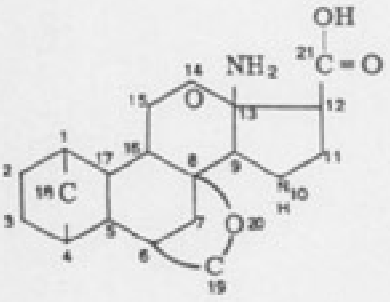
(3)



(4)



(5)



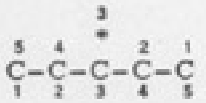
Formula (5) illustrates that the enumeration pattern of an unsymmetrical substituent free ring system holds for the substituted system regardless of the nature or distribution of acyclic skeletal substituents or ring bridges.

2.6 MOLECULES HAVING SYMMETRICAL PATHS IN THE SATURATED HYDROCARBON STATE

Whenever a molecule in the virgin state contains carbon paths which are symmetrical with respect to a point in the molecule so that the order of enumeration of such paths with respect to one another is arbitrary, the enumeration pattern thereof is not unique, but is unambiguous in the sense that any one of the equivalent enumeration patterns of the paths concerned will yield the same cipher (and same name).

EXAMPLES (asterisks mark points of symmetry):

(1)



$$\underset{1}{\overset{5}{C}}-\underset{2}{\overset{4}{C}}-\underset{3}{\overset{\overset{3}{*}}{C}}-\underset{4}{\overset{2}{C}}-\underset{5}{\overset{1}{C}}$$

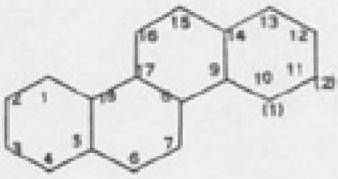
cipher: C5 See 2.8 TABLE I.

(2)

$$\underset{1}{\overset{6}{C}}-\underset{2}{\overset{5}{C}}-\underset{3}{\overset{4^{*}}{C}}-\underset{4}{\overset{3}{C}}-\underset{5}{\overset{2}{C}}-\underset{6}{\overset{1}{C}}$$

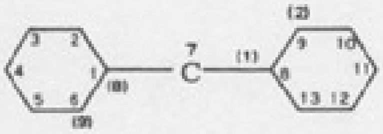
cipher: C6

(3)



cipher: $6\overset{1}{L}4\overset{5}{Y}LL\overset{8}{Y}\overset{9}{Y}L4YLLYY$ See 2.8, I.

(4).



cipher: 6L(C@6LL5)L5

When the paths just described are made unsymmetrical by one or more derived features, the order of enumeration can no longer be arbitrary since ambiguities would thereby infiltrate the enumeration pattern. The following rule, which may be called the "updating rule", serves to monitor the imposition of derived features upon arbitrarily enumerated symmetrical paths of the parent saturated hydrocarbon so as to ensure that the enumeration pattern will remain unambiguous (or become unique) and be completely congruent, at all stages of derivation, with the enumeration pattern of the saturated parent hydrocarbon.

2.61 UPDATING RULE:

When paths which are symmetrical with respect to a point in a saturated hydrocarbon so that the order of enumeration of such paths is arbitrary are made unsymmetrical by one or more derived features, enumerate such paths in the order in which the ascending enumeration pattern assigns the lower number on the occasion of the first difference to the following features listed in their order of decreasing priority:

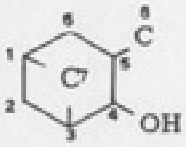
1. heavier skeletal atom;
2. skeletal atom to which is bonded the
   a. greater number of functional substituents;
   b. heavier functional substituent;
   c. more unsaturated skeletal bond.

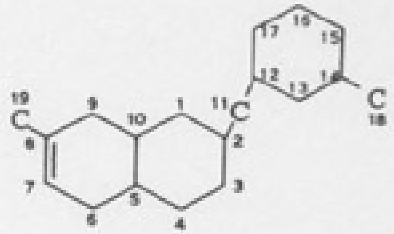
It will be noted that none of the above features introduces additional skeletal atoms into the basic structure. See Sec. 1.2.

In the case of ring compounds, wherein the basic structure for beginning the enumeration is always an unsubstituted saturated hydrocarbon ring system, it is possible that carbon paths which are symmetrical in the basic ring system may be made unsymmetrical by the introduction of skeletal substituents of the following types:

1. ring bridges;
2. skeletal substituents attached to ring by acyclic bonding.

EXAMPLES:





In all such cases the enumeration logic ensures that the enumeration pattern of any ring compound will always be congruent with that of the saturated hydrocarbon ring system with which the enumeration of such compound begins, as will be set forth in Sections 4 to 7.

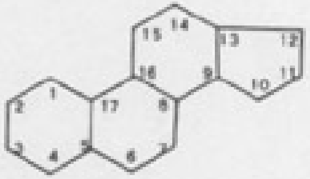
2.7 GENERAL CIPHERING ORDER

Cipher serially bonded paths of atoms of unbroken numerical sequence and atoms of the same discrete ring system, excluding bridges, in their ascending numerical order, except that all substituents of a given atom must be ciphered before ciphering the next configuration of the parent path to which such given atom belongs. See also rule 3 of Sec. 2.8.

(1)

C6

(2)



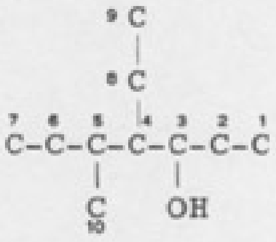
$\mathrm{\overset{1}{L}4\overset{5}{Y}\overset{6}{L}\overset{7}{L}\overset{8}{Y}\overset{9}{Y}5L3\overset{13}{Y}LL\overset{16}{Y}\overset{17}{Y}}$

2.8 ORDER OF CIPHERING SUBSTITUENTS

1. Cipher substituents groups (See Sec. 1.4 and 1.5) directly after ciphering their related parent atoms and before ciphering the next higher numbered atom or intervening multiple bond in the parent path.

EXAMPLE:

(1)



Cipher: $\mathrm{ECQ\overset{4}{C}EC\overset{10}{M}E}$

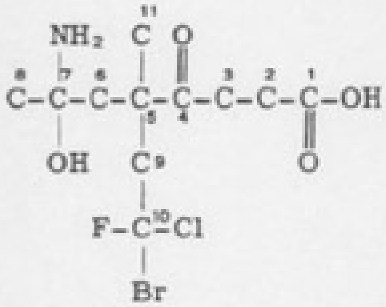
2. When a plurality of different substituent groups are attached to the same parent atom, cipher such groups, consistent with rules 3-5 below, in the following order of decreasing priority:

(1) functional substituents (in the order of their increasing weights-lightest first-when there is a plurality)

(2) skeletal substituents (in their ascending numerical order-lowest numbered group first-when there is a plurality)

EXAMPLES:

(2)



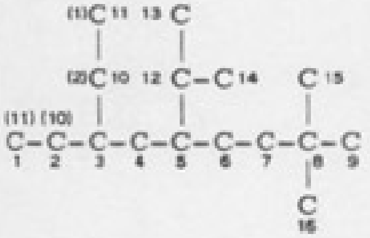
Cipher: CVQCCCVC(CCFKB)MCCZQM

3. When one or more acyclic substituent groups of a given parent atom is the same as the group which begins or terminates the parent path concerned, cipher one of such groups* as a substituent of the parent atom in question and multiply the cipher of such group by a number equal to the total number of its occurrences, unless the group is a methyl group of the isopropyl radical which is always represented by the symbol "T."

When one of the groups described begins the enumeration, cipher such groups after the parent atom to which commonly bonded and before ciphering any other skeletal configuration attached to such parent atom. Any functional substituent attached to the same parent atom as the enumerated (skeletal) groups just described is ciphered before the latter groups as required by item 2, above.

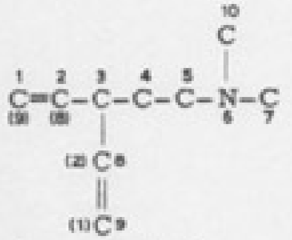
EXAMPLES:

(1)



$\mathrm{\overset{3}{C}E2\overset{4}{C}CTCC\overset{7}{C}M3}$

(2)

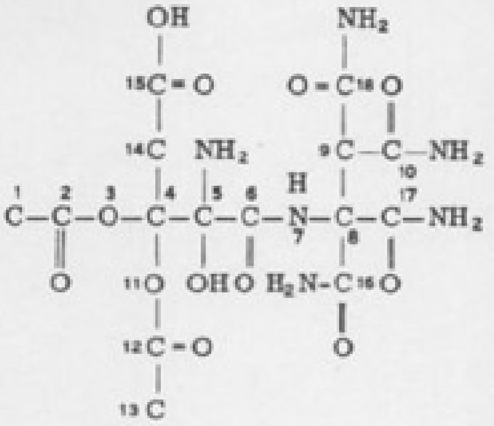


$\mathrm{\overset{3}{C}(C{=}C)2\overset{4}{C}C\overset{6}{N}M2}$

---

* The lowest numbered group if skeletal

(3)



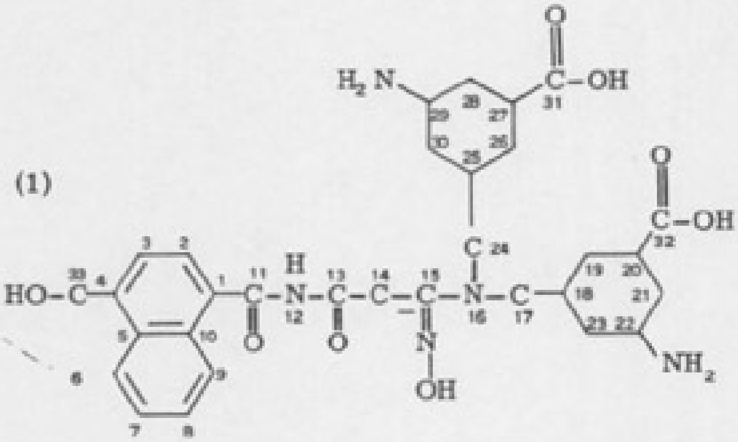
$\overset{4}{\mathrm{C}}$(OCVM)2(CCVQ)$\overset{5}{\mathrm{C}}$ZQ$\overset{6}{\mathrm{C}}$VNH$\overset{8}{\mathrm{C}}$(CVZ)2$\overset{9}{\mathrm{C}}$(CVZ)2

4. When a substituent group differs from the type described by item 3 above only in that such group contains a ring, cipher the groups in the same manner prescribed by item 3 above when such groups terminate a parent path.

When one of such ring containing groups begins the enumeration, do not include such group in a multiplied cipher since the cipher must begin with atom "1" of the generating ring system prefixed by the size of the ring containing atom "1", as set forth in Section 7. See NOTE below.

EXAMPLES:

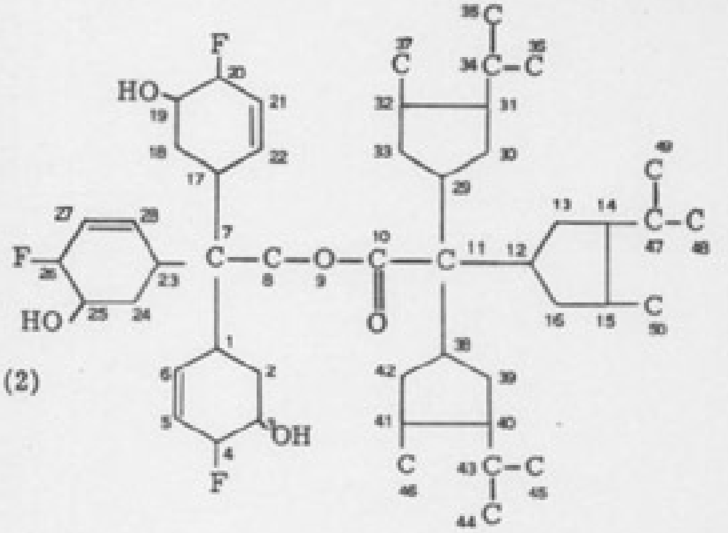
(1)



6$\overset{1}{\mathrm{R}}$($\overset{11}{\mathrm{C}}$VNHCVC$\overset{15}{\mathrm{C}}$(=NQ)$\overset{16}{\mathrm{N}}$(C@6LLL(CVQ)LLZL)2$\overset{2}{\mathrm{R}}$RR

(CQ)$\overset{5}{\mathrm{Y}}$NRRR$\overset{10}{\mathrm{Y}}$

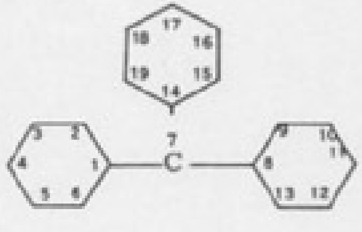
(2)



$\overset{1}{6}$L($\overset{7}{\mathrm{C}}$(@6LLLQLFL:L)2$\overset{8}{\mathrm{C}}$O$\overset{10}{\mathrm{C}}$V$\overset{11}{\mathrm{C}}$@5LLLTLML)$\overset{2}{3}$)LLQ

$\overset{4}{\mathrm{L}}$FL:$\overset{6}{\mathrm{L}}$

NOTE. The mechanical analysis method of Isaacs and Walker (15) relies upon the presence or absence of an arabic numeral as the first character of a cipher-except that of a salt-to establish whether the cipher is that of an acyclic compound or of a cyclic compound. In cases such as the following,



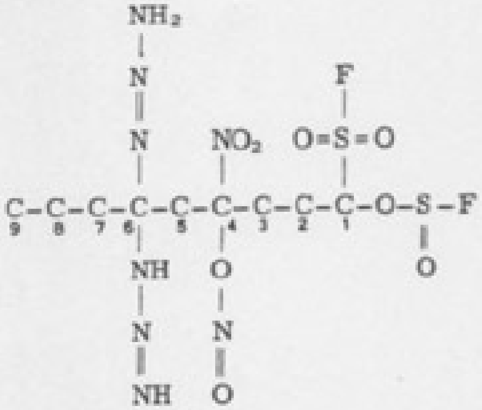
in the absence of the exception defined by rule 4, the first character of the cipher, as of the above compound "C(@6LL5)3", could not be relied upon for the purpose stated. It is a present feature of the system that the ciphers of all ring containing compounds must begin with a number equal to the size of the ring which begins the enumeration.

5. When a plurality of functional substituents which have the same weight but different chemical configurations are attached to the same parent atom, cipher the substituents in the order in which there is generated from the parent atom into the respective substituents either the

(1) First lighter substituent atom, or the

(2) first more saturated substituent bond, whichever is generated earlier, according to the procedure for generating the atoms and bonds of functional substituents as described in Sec. 3.6.

EXAMPLE:



Cipher: $\overset{1}{C}$ (OSVF) (SWF) CC$\overset{4}{C}$ (NW) (ONV) C$\overset{6}{C}$ (NHN=NH) (N=NZ) C3

2.9 TABLE OF SYMBOLS.

TABLE I—Symbols for Carbon and Hydrogen

Symbol For

C—Acyclic carbon atoms and carbon atoms which serve as connecting links between component ring systems of a circular ring assembly except acyclic carbon atoms which

1. are otherwise expressed as a methyl "M", ethyl "E", or isopropyl "T" group.
2. are included in a multipliable series of three or more chain units attached to carbon only, as explained in TABLES VI and VII B.

E—Ethane when used alone; otherwise ethyl, $-CH_2CH_3$ only; not used when bonded to a methylene $-CH_2-$ unit in which case the group is expressed as a series, as explained in TABLE VII B; E is used to express a carry over series of two which terminates an alkyl chain. See TABLE VII footnote.

L—Unfused* carbon atom of "L"-type* ring when such atom is not included in a multipliable series of three or more methylene $-CH_2-$ring units attached only to carbon as explained in TABLE VII B. See "(L)" TABLE VIII.

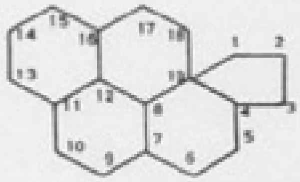
M—Methane when used alone; otherwise methyl, $-CH_3$ only; not used when bonded to a methylene $-CH_2-$ unit in which case the group is expressed either by "E" (ethyl) or by a multiplied series, whichever applies as explained above; not used for the methyl groups of isopropyl which latter group is always expressed by "T".

R—Unfused carbon atom of "R"-type* ring when such atom is not included in a multipliable series of three or more methine ($-CH=$, or $=CH-$) ring units attached only to carbon, as explained in TABLE VII B. See (R) TABLE VIII.

T—Propane when used alone; otherwise isopropyl, $-CH(CH_3)_2$ only.

X—Spiro-fused* carbon atom; suffixed by an arabic numeral equal to the size of the ring, if other than 6 - membered, when the X symbol represents the first ciphered atom of such ring. See also the dash symbol "-" TABLE IX and the symbol "(X)" TABLE II.

Y—Ortho-fused* carbon atom which is common to not more than two ortho-fused faces, i.e. peripheral, as illustrated by atoms 4, 7, 11, 16, and 19 in the structural formula immediately below. See Section 5.02 for geometric significance of Y and y symbols and suffixes denoting ring sizes. See TABLE II for (Y).



y—Interior ortho-fused* atom, common to at least three ortho-fused faces, as illustrated by atoms 8, and 12 in the formula immediately above; suffixed by size of ring embraced by arms of y (Sec. 5.02) if other than 6-membered. See TABLE II for (y).

H—Hydrogen atom bonded to an atom other than carbon, except for H of OH and NH_2 groups; hydrogen atoms bonded to carbon are not ciphered but implied; hydrogen atom of hydroxy "OH" and primary amino "NH_2" groups is expressed by the composite symbols for such groups, viz: Q and Z respectively; stereochemical configuration of a hydrogen atom which lies on the opposite side of ring plane from reference group and is bonded to ortho-fused atom is denoted by the symbol "a" after the Y symbol representing the ortho-fused atom, the "a" following the ring size when cited.

---

*See Sections 1.9 and 5.0

TABLE II—Symbols for Oxygen, Nitrogen, Sulfur, Phosphorus, and the Halogens

Symbol For

B—bromine atom; Boron symbol changed to [BO].

F—fluorine atom.

G—halogen (See TABLE VIII).

I—iodine atom.

K—chlorine atom.

N—acyclic nitrogen atom and a nitrogen atom of a ring of rings, which atom is not included in a component ring system thereof, when the nitrogen atom does not comprise a primary amino, NH_2, group.

n—nitrogen atom of a ring or ring bridge, except a nitrogen atom of a ring of rings which is not included in one of the component ring systems (See "N" above); not multipliable in a series.

O—oxygen atom which interrupts a carbon chain or ring.

P—phosphorus atom.

Q—OH, hydroxy group; multiplied by appropriate numerical suffix to denote a plurality of such groups attached to same parent atom.

S—sulfur atom.

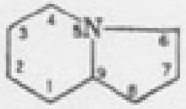
V—=O, "oxo" group (oxygen atom bonded solely to one other atom to which no other oxygen atom is solely bonded).

W—=O,=O, "gem. dioxo" (two oxygen atoms bonded solely to the same other atom); considered as a set of two oxo substituents in determining the order of enumeration of derived paths and the order of ciphering a plurality of functional substituents bonded to the same parent atom.

Z—NH_2 "primary amino" group; the $-\overset{H}{\underset{H}{N}}-$ configuration of an amine addition salt is ciphered by "NH2", amine addition salts and quaternany ammonium salts being ciphered without any special symbology to denote "onium" character which is represented implicitly by the manner of ciphering salts.

(X), (Y), (y) . . .

When a hetero atom occupies an ortho-fused or spiro-fused position, cipher such atom by its assigned symbol and follow the symbol immediately by the cipher of a carbon atom (enclosed by parentheses) as if the carbon atom occupied the same position, including ring sizes if required (See TABLE I, X, Y, y.). For example, position "5" of the formula below



is represented by n(Y5).

The "dummy", or "shadow", cipher of the fictitious carbon atom facilitates deciphering and permits the number and kind of fusion points to serve as a screen, if desired, for file organization and searching operations.

TABLE III—Symbols of Elements Not Included in Tables I and II

The international letter symbols of the elements listed below have been changed, as indicated, so that the single character symbols may represent atoms or groups which have high frequency of occurrence in organic compounds (See the discussion by WISWESSER, cited in the introduction), and so that the symbols of all elements other than those included in TABLES I and II will have the same number of characters.

Element	International symbol	Notation symbol
ARGON	A	[AR]
BORON	B	[BO]
POTASSIUM	K	[KA]
URANIUM	U	[UR]
VANADIUM	V	[VA]
TUNGSTEN	W	[WO]
YTTRIUM	Y	[YT]

All of the remaining elements which are not represented above or in TABLES I and II are ciphered by the international symbols in capital letters enclosed by brackets, as illustrated above.

TABLE IV—Symbols for Bonds

Symbol	For
= (equality sign)	—acyclic double bond-cis, trans relation unspecified.
: (colon)	—double bond of "L" ring-cis trans relation unspecified.
÷ (division sign)	—triple bond (ring or chain)
(=)	—cis double bond of open chain or of connecting chain of a circular ring assembly.
[=]	—trans double bond of open chain or of connecting chain of a circular ring assembly.
(:)	—cis double bond of "L" ring.
[:]	—trans double bond of "L" ring.
{:}, or +:+	—double bond of ortho-fused face which is not part of an "R" ring; ciphered only after the lower numbered atom to which attached; follows ring size numeral where cited.

TABLE V—Symbols for Steric Relationships

Symbol	For
a	—as suffix to denote that the preceding substituent lies on the opposite side "anti" of the ring plane from the reference group. —See also Section 8.6.
(+)	—as final item of the cipher to denote optical activity of a <u>dextrorotatory</u> nature.
(-)	—optically active <u>levorotatory</u> compound; final item of cipher.
(+-)	—optically inactive <u>racemic</u> mixture; final item of cipher.
(-+)	—optically inactive <u>meso</u> compound; final item of cipher.
(=)	—"cis" double bond of chain (including "chain" portion of a circular assembly.
[=]	—"trans" double bond of chain (including chain portion of a circular ring assembly.
(:)	—"cis" double bond of ring.
[:]	—"trans" double bond of ring.

TABLE VI—Enclosure Symbols. Parentheses, ( ); Brackets, "[ ]"; Braces, "{ }"

Symbol	Use
( )	—to enclose the cipher of any substituent whose cipher contains more than one character or a multiple there of, e.g. M2. To denote a plurality of such a substituent attached to the same atom suffix the closing parenthesis by a number equal to the number of occurrences of such substituent. See TABLE VII and Section 2.8. To enclose a bridge identifying number, e.g. (2) SEE TABLE VII and 6.1. See TABLE IV for (=) and (:). See TABLE IX for (@) and ( ). See TABLE V for (+), (-), (+-), (-+).
[ ]	—to enclose the letters which represent elements as indicated in TABLE III. To enclose ions. See TABLE IV for [=] and [:].
{ } or ++	—to enclose repeating non-terminal units of a chain, other than methylene units, when three or more; suffix the closing brace by a number equal to the number of units in the series; a <u>series of three or more unsubstituted hetero atoms</u> in a chain is denoted by ciphering the atom once and multiplying the atom symbol by the appropriate numerical suffix. See TABLE IV for {:}.

TABLE VII—Arabic Numerals

Symbol	For
Δ	zero
1	one
2	two
3	three
4	four
5	five
6	six
7	seven
8	eight
9	nine
?	indefinite number or position.

A. The appropriate arabic numeral is used as a prefix before:

(1) the first symbol of the compound cipher, when such symbol represents a ring atom, to denote the size of the ring which contains said ring atom. (See 4.2).

(2) the symbol of the first ciphered atom of a component ring system, other than the generating ring system, of a ring assembly to denote the size of the ring which contains said first ciphered ring atom; ring size number substituted by a question mark "?" when said first ciphered atom comprises a ring bridge.

(3) the introductory bracket of an ion cipher to denote the number of occurrences of the ciphered ion in the ciphered salt. (See 10.2(2)).

B. The appropriate arabic numeral is used as a suffix after:

(1) the symbol "c" to denote a series of three to nine* methylene "$-CH_2-$" units in a chain when the terminal bonds of the series are attached only to carbon, include any methyl group which begins or terminates such a series in the series, e.g. $-CH_2CH_2CH_3$ is ciphered "C3".

(2) the symbol "L" to denote a series of three to nine* methylene "$-CH_2-$" units in a ring when the terminal bonds of the series are attached only to carbon (See 4.2).

(3) the symbol "R" to denote a series of three to nine* methine "$=CH-$ or $-CH=$" units in a ring when the terminal bonds of the series are attached only to carbon (See 4.2).

(4) the symbol of a hetero atom to denote a series of three to nine* unsubstituted bivalent hetero atoms in a chain.

(5) the closing parenthesis of a substituent cipher to denote the number of occurrences when a plurality of the parenthesized substituent is bonded to the same atom. (See 2.8 rules 3 and 4).

(6) any one of the symbols A, B, E, F, G, H, I, K, M, Q, T, Z to denote the number of occurrences when a plurality of the substituent represented is bonded to the same atom, except the methyls which comprise the isopropyl group which is always ciphered by T.

(7) the symbol "Y" to denote the size of the ring (when other than 6-membered) which is embraced by the "arms" of the Y (See TABLE I, Y and 5.02).

(8) the symbol "y" to denote the size of the ring (when other than 6-membered) which is embraced by the "arms" of the y (See TABLE I, y) and 5.02.

(9) the symbol "X" to denote the size of the ring (when other than 6-membered) of which the X symbol represents the first ciphered atom (See 5.5(3)).

(10) the closing bracket symbol "]" to denote the number of electrovalences (charges) associated with the bracketed ion (See 10.2(4)).

(11) the closing brace symbol "}" to denote a series of three to nine* repetitive units of a chain when the unit consists of at least two atoms and is not a methylene unit (See 3.7(11)).

The appropriate arabic numeral enclosed by parentheses is used to terminate the cipher of each path of bridge atoms and to serve as an identifying number which is repeated, also parenthesized, immediately after the highest numbered

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When the number of units in the series described by (1), (2), (3), and (4), above, exceeds nine denote the units in excess of nine by successive series of nine units each and/or by a "carry over" series of less than nine, or "CC", C, E, or M, to exhaust the series. When the number of units in a series of repetitive chain units (which may include repeating ring systems) of the type described by (11) above, exceeds nine increase the value of the numerical suffix by one for each additional unit in the series without upper limit. If the number of repetitive units is unknown suffix the closing brace by a question mark "?" to indicate that the number is indefinite. See 9.2(1).

parent ring atom to which the identified bridge or bridge branch is connected but after the ring size where cited. Beginning with the combination symbol "(1)" to identify the end of the first bridge path increase the number by one for each sucessive bridge ending which does not terminate at an already identified bridgehead. See 6.6-6(2).

The zero symbol " " is used to suffix the symbol of a bridge atom from which a plurality of bridge paths branch. The branches are enumerated and ciphered in the ascending numerical order of the parent ring atoms at which such branches terminate. See 6.6-4a.

TABLE VIII—Generic Symbols. "r" Symbol. Unassigned Symbols D, J, and U

Symbol	Use
A	—to represent the term "alkyl" when no species is designated.
D	—unassigned.
G	—to represent halogen when no species is designated.
J	—unassigned.
U	—unassigned.
r	—placed after the first ciphered atom of an "R" ring of which none of the atoms is represented by an "R" symbol to indicate that the ring is of the "R" type; absence of an "r" after the first ciphered atom of a ring none of whose atoms is represented by an "L" or "R" symbol indicates the ring to be of the "L" type (See Sec. 1.9 for definition of "R" ring and "L" ring).
(R)	—to represent the term "aryl" when no species is designated.
(L)	—to represent the term "alicyclic", or "cycloaliphatic", when no species is designated.
(H)	—to represent the term "heterocyclic" when no species is designated.
A(R)	—to represent the term "alkaryl", or "alkylaryl" when no species is designated.
(R)A	—to represent the term "aralkyl", or "arylalkyl", when no species is designated.

TABLE IX—Miscellaneous Non-Letter Symbols

Symbol	Use
* (asterisk)	—as dummy symbol to introduce bridge; placed before first symbol of bridge cipher.
- (dash)	—as dummy symbol to indicate skipping over an already ciphered ring atom, as in the case of a spiro atom, when a skip is required to access the next high-numbered unciphered ring atom.
; (semi-colon)	—to separate anion(s) cipher(s) from cation(s) cipher(s) in the cipher of a salt.
, (comma)	—to separate the ciphers of ions of like charge where a plurality of such ions exist in the same salt. —to separate ring size numbers which follow a Y or y symbol (See TABLE I, Y, y). —to prefix the cipher of an interior atom of a fused ring aggregate when such atom is not part of a peripheral ring.
? (question mark)	—suffix after closing brace " } " to denote that the embraced chain unit is polymeric; suffix after the symbol "@" to indicate that the next ciphered atom is an atom of a ring bridge.
(period)	—to introduce cipher of acyclic carbon - containing substituent (group which breaks the ascending sequence of numbers); used for mechanical retrieval purposes. Chelate designation. See Section 10.5.

Symbol	Use
¢ (cent sign)	—to close cipher of acyclic carbon - containing substituent; used for mechanical retrieval purposes.
! (exclamation point)	—to introduce cipher of ring-containing substituent (group which breaks the ascending sequence of numbers and contains a ring); used for mechanical retrieval purposes.
$ (dollar sign)	—to close cipher of ring-containing substituent; used for mechanical retrieval purposes.
# (sharp)	—reserved for mechanical "housekeeping"
% (per cent)	—reserved for mechanical "housekeeping"
/ (slanted stroke)	—to separate cipher of terminal ring and substituents thereof from cipher of repeating middle portion of polymer. See Section 9.3.
@	—to introduce a component ring system of a ring assembly; immediately precedes first ciphered atom o introduced system if ring containing such atom is 6-membered (See Section 7-); precedes ring size numeral which is cited whenever such ring is other than 6-membered (See Section 7); precedes ? when used to indicate bridge atom. See IX.
@)	—to indicate point where substituent portion (See Sec. 7) of a circular assembly connects to generating ring system so as to form a ring of rings; placed after symbol of substituent atom, or bond if multiple, which is directly connected to generating ring system.
( )	—to indicate point on generating ring system of a closed ring assembly to which the "tail end" of the substituent portion is connected; placed immediately after that atom of the generating ring system to which the "tail end" of the substituent portion is bonded.

TABLE X—Common Functional Substituents Arranged in Alphabetical Order of Ciphers

Cipher	Substituent	Weight
1. B	-Br	79.916
2. F	-F	19.000
3. I	-I	126.910
4. (IV)	-IO	142.910
5. (IW)	$-IO_2$	158.910
6. K	-Cl	35.457
7. (+N)	≡N	14.008
8. (=NH)	=NH	15.016
9. (NHNHZ)	$-NHNHNH_2$	46.056
10. (NHN=NH)	-NHN=NH	44.040
11. (NHPVZ2)	$-NHP{=}O(NH_2)_2$	94.039
12. (NHPZ2=S)	$-NHP{=}S(NH_2)_2$	110.105
13. (NHZ)	$-NHNH_2$	31.040
14. (N=NH)	-N=NH	29.024
15. (N=NZ)	$-N{=}NNH_2$	44.040
16. (=NQ)	=NOH	31.016
17. (NV)	-NO	30.008
18. (NW)	$-NO_2$	46.008
19. (=NZ)	NNH_2	30.032
20. (ONV)	-ONO	46.008
21. (ONW)	$-ONO_2$	62.008
22. (OOPVQ2)	$-OOP{=}O(OH)_2$	112.991
23. (OOSWQ2)	$-OOSO_2OH$	113.074
24. (OPQB)	-OP(OH)Br	143.899
25. (OPQF)	-OP(OH)F	82.983
26. (OPQI)	-OP(OH)I	190.893
27. (OPQK)	-OP(OH)Cl	99.440
28. (OPQ2=S)	$-OP{=}S(OH)_2$	113.057
29. (OPVB2)	$-OP{=}OBr_2$	222.807
30. (OPVF2)	$-OP{=}OF_2$	100.975
31. (OPVI2)	$-OP{=}OI_2$	316.795
32. (OPVK2)	$-OP{=}OCl_2$	133.889
33. (OPVQ2)	$-OP{=}O(OH)_2$	96.991
34. (OPVQOPVQ2)	$-OP{=}O(OH)OP{=}O(OH)_2$	176.974
35. (OPVZ2)	$-OP{=}O(NH_2)_2$	95.023
36. (OPVZQ)	$-OP{=}ONH_2OH$	96.007
37. (OQ)	-OOH	33.008
38. (OSH)	-OSH	49.074
39. (OSVB)	-OS=OBr	143.982

Cipher	Substituent	Weight
40. (OSVF)	-OS=OF	83.066
41. (OSVI)	-OS=OI	190.976
42. (OSVK)	-OS=OCl	99.523
43. (OSVQ)	-OS=OOH	81.074
44. (OSWB)	$-OSO_2Br$	159.982
45. (OSWF)	$-OSO_2F$	99.066
46. (OSWI)	$-OSO_2I$	206.976
47. (OSWK)	$-OSO_2Cl$	115.523
48. (OSWOSWQ)	$-OSO_2OSO_2OH$	177.140
49. (OSWQ)	$-OSO_2OH$	97.074
50. (=PH)	=PH	31.983
51. (PH2)	$-PH_2$	32.991
52. (PQ2)	$-P(OH)_2$	64.991
53. Q	-OH	17.008
54. (=S)	=S	32.066
55. (SB)	-S-Br	111.982
56. (SF)	-S-F	51.066
57. (SH)	-SH	33.074
58. (SI)	-S-I	158.976
59. (SK)	-S-Cl	67.523
60. (SSH)	-SSH	65.140
61. (SVB)	-S=OBr	127.982
62. (SVF)	-S=OF	67.066
63. (SVI)	-S=OI	174.976
64. (SVK)	-S=OCl	83.523
65. (SVQ)	-S=O(OH)	65.074
66. (SVZ)	$-S=ONH_2$	64.090
67. (SWB)	$-SO_2Br$	143.982
68. (SWF)	$-SO_2F$	83.066
69. (SWI)	$-SO_2I$	190.976
70. (SWK)	$-SO_2Cl$	99.523
71. (SWQ)	$-SO_2OH$	81.074
72. (SWZ)	$-SO_2NH_2$	80.090
73. V	=O	16.000
74. W	=O , =O	16.000
75. Z	$-NH_2$	16.024

TABLE XI--Common Functional Substituents Arranged in Order of Increasing Weight

Substituent	Weight	Cipher
1. ≡N	14.008	1. (+N)
2. =NH	15.016	2. (=NH)
3. =O or =O, =O (W)	16.000	3. V
4. $-NH_2$	16.024	4. Z
5. -OH	17.008	5. Q
6. -F	19.000	6. F
7. -N=NH	29.024	7. (N=NH)
8. -NO	30.008	8. (NV)
9. $=NNH_2$	30.032	9. (=NZ)
10. =NOH	31.016	10. (=NQ)
11. $-NHNH_2$	31.040	11. (NHZ)
12. =PH	31.983	12. (=PH)
13. =O, =O See =O	32.000 (16+16)	13. W
14. =S	32.066	14. (=S)
15. $-PH_2$	32.991	15. (PH2)
16. -OOH	33.008	16. (OQ)
17. -SH	33.074	17. (SH)
18. -Cl	35.457	18. K
19. $-N=NNH_2$*	44.040	19. (N=NZ)
20. -NHN=NH*	44.040	20. (NHN=NH)
21. $-NO_2$*	46.008	21. (NW)
22. -ONO*	46.008	22. (ONV)
23. $-NHNHNH_2$	46.056	23. (NHNHZ)
24. -OSH	49.074	24. (OSH)
25. -SF	51.066	25. (SF)
26. $-ONO_2$	62.008	26. (ONW)
27. $-S=ONH_2$	64.090	27. (SVZ)
28. $-P(OH)_2$	64.991	28. (PQ2)
29. -S=OOH	65.074	29. (SVQ)
30. -SSH	65.140	30. (SSH)
31. -S=OF	67.066	31. (SVF)
32. -SCl	67.523	32. (SK)
33. -Br	79.916	33. B
34. $-SO_2NH_2$	80.090	34. (SWZ)
35. $-SO_2OH$	81.074	35. (SWQ)
36. -OP(OH)F	82.983	36. (OPQF)
37. -OS=OF*	83.066	37. (OSVF)
38. $-SO_2F$*	83.066	38. (SWF)
39. -S=OCl	83.523	39. (SVK)
40. $-NHP=O(NH_2)_2$	94.039	40. (NHPVZ2)
41. $-OP=O(NH_2)_2$	95.023	41. (OPVZ2)
42. $-OP=O(OH)NH_2$	96.007	42. (OPVZQ)
43. $-OP=O(OH)_2$	96.991	43. (OPVQ2)
44. $-OSO_2OH$	97.074	44. (OSWQ)
45. $-OSO_2F$	99.066	45. (OSWF)
46. -OP(OH)Cl	99.440	46. (OPQK)
47. -OP(OH)Cl	99.440	47. (OPQK)
48. $-OP=OF_2$	100.975	48. (OPVF2)
49. $-NHP=S(NH_2)_2$	110.105	49. (NHPZ2=S)
50. -SB	111.982	50. (SB)
51. $-OOP=O(OH)_2$	112.991	51. (OOPVQ2)
52. $-OP=S(OH)_2$	113.057	52. (OPQ2=S)
53. $-OOSO_2OH$	113.074	53. (OOSWQ)
54. $-OSO_2Cl$	115.523	54. (OSWK)
55. -S=OBr	127.982	55. (SVB)
56. $-OP=OCl_2$	133.889	56. (OPVK2)
57. -IO	142.910	57. (IV)
58. -OP(OH)Br	143.899	58. (OPQB)
59. -OS=OBr*	143.982	59. (OSVB)
60. $-SO_2Br$*	143.982	60. (SWB)
61. $-IO_2$	158.910	61. (IW)
62. -SI	158.976	62. (SI)
63. $-OSO_2Br$	159.982	63. (OSWB)
64. -S=OI	174.976	64. (SVI)
65. -OP=O(OH)OP	176.974	65. (OPVQOPVQ2)

Substituent	Weight	Cipher
66. -OSO_2OSO_2OH	177.140	66. (OSWOSWQ)
67. -OP(OH)I	190.893	67. (OPVI)
68. -SO_2I	190.976	68. (SWI)
69. -OSO_2I	206.976	69. (OSWI)
70. -$OP{=}OBr_2$	222.807	70. (OPVB2)
71. -$OP{=}OI_2$	316.795	71. (OPVI2)

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*See resolution of isobaric (same weight) substituents attached to same atom as set forth in section 3.61.

TABLE XII—Summary of Single Character Symbols

Symbol Principal Assignment	See Table	See Compound
1. A—Alkyl	VII, VIII	
2. a—"trans" suffix	V	8.41(2)
3. B—bromine	II, VII	3.6(3)
4. C—chain carbon	I, VII	3.3(1)
5. D—unassigned	VIII	
6. E—ethyl	I, VII	3.3(1)
7. F—fluorine	II, VII	3.6(3)
8. G—halogen	II, VII, VIII	
9. H—hydrogen, attached to hetero (except OH and NH_2)	I, VII, VIII	3.7(3)
10. a—hydrogen, stereochemical	I, V	8.42(1)
11. I—iodine	II, VII	3.6(6)
12. J—unassigned	VIII	
13. K—chlorine	II, VII	3.6(1)
14. L—"L" ring carbon	I, VII, VIII	4.2(8)
15. M—methyl	I, VII	3.3(3)
16. N—chain nitrogen	II	3.7(3)
17. n—ring nitrogen	II	4.2(8)
18. O—ring or chain oxygen	II	3.7(2)
19. P—phosphorus	II	3.62(8)
20. Q—OH (hydroxy)	II, VII	3.6(4)
21. R—"R" ring carbon	I, VII, VIII	4.2(9)
22. r—to denote "R" ring containing no "R" atom	VIII	5.56(1)
23. S—sulfur	II	3.7(5)
24. T—isopropyl	I, VII	3.3(1)
25. U—unassigned	VIII	
26. V—=O (oxo)	II	3.7(5)
27. W—=O,=O (gem. dioxo)	II	3.7(5)
28. X—spiro carbon	I	5.41(9)
29. Y—peripheral ortho-fused atom	I	5.22(1)
30. y—interior ortho-fused atom	I	5.22(1)
31. Z—NH_2 (primary amino)	II, VII	3.7(15)
32. Δ—zero, bridge branch	VII	6.6-42
33. 1—one	VII	
34. 2—two	VII	
35. 3—three	VII	
36. 4—four	VII	
37. 5—five	VII	
38. 6—six	VII	
39. 7—seven	VII	
40. 8—eight	VII	
41. 9—nine	VII	
42. (—substituent enclosure	VI, IV, VII	3.6(7)
43.)—substituent enclosure	VI, IV, VII	3.6(7)
44. [—ion enclosure	VI, IV	10.2(1)
45.]—ion enclosure	VI, IV	10.2(1)
46. {—repetitive chain unit enclosure	VI, IV	3.7(11)
47. }—repetitive chain unit enclosure	VI, IV	9.2(1)
48. =—chain double bond	IV, V	3.5(1)
49. :—"L" ring double bond	IV, V	4.2(8)
50. ÷—triple bond	IV	3.5(5)
51. ;—to separate ions of unlike charge	IX	10.2(1)
52. ,—to separate ions of like charge	IX	10.2(5)
53. ?—indefinite number or position	IX, VII	9.3(1)
54. /—to segregate part of polymer cipher	IX	9.3(1)
55. *—to introduce bridge	IX	11.0(3)
56. @—to introduce component ring system	IX	11.0(4)
57. - —to skip over already ciphered ring atom	IX, V	5.4(3)
58. + —dextrorotatory	V	8.8(2)
59. . —chelate designation	IX	10.5(2)
60. ¢—reserved for IR	IX	
61. !—reserved for IR	IX	
62. $—reserved for IR	IX	
63. #—reserved for "housekeeping"	IX	
64. %—reserved for "housekeeping"	IX	

TABLE XIII—Summary of Multiple Character Symbols Which Contain No Letters

Symbol	Assignment	See Table	See Compound
(=)	cis double bond (chain)	IV	8.03(2)
[=]	trans double bond (chain)	IV	8.03(1)
(:)	cis double bond (ring)	IV	8.2(1)
[:]	trans double bond (ring)	IV	8.2(2)
(;)	double bond of fused face which is not part of an "R" ring.	IV	5.55(1)
(+)	dextrorotatory	V	8.8(2)
(-)	levorotatory	V	8.8(1)
(+-)	racemic	V	
(-+)	meso	V	8.8(3)
@)	end of substituent portion of a ring of rings.	IX	7.8(1)
( )	point on generating ring where tail end "@" of substituent portion is attached.	IX	7.8(1)

3.0 ACYCLICS. BRANCHING PATHS

Acyclic molecules are the simplest of all organic molecules and establish the only class whose members can be described geometrically by either a straight line or a system of straight lines. The problem presented to enumeration and line formula notation by the geometry of Acyclics, as well as of Monocyclics and Fused Ring Aggregates, is branching in the reference plane, since each notated position (atom) from which a plurality of different paths diverge exacts a decision as to the order of enumeration and of ciphering the paths involved.

The enumeration of an acyclic compound begins always with a terminal carbon atom and follows branching directions wherever encountered according to the rules set forth in the following section. That terminal carbon which generates the sequential enumeration pattern which assigns the lower number on the occasion of the first difference to the structural features listed in Section 3.2 in their order of decreasing priority is the correct starting atom.

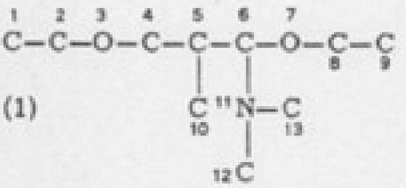
3.1 ORDER OF ENUMERATION OF ACYCLIC COMPOUNDS

Each terminal carbon atom is a potential starting atom. The correct enumeration pattern is derived by a process of competitive enumeration and elimination according to the following procedure:

1. Beginning with a terminal carbon atom as atom "1" enumerate sequentially along the chain, skeletal atom (see sec. 1.3 for definition) by skeletal atom, until an atom is enumerated, if any, from which unenumerated skeletal paths branch.
2. Continue to enumerate along that branch, and along each successive branch encountered, which exhibits the following features in the order of decreasing priority the
    a. greater number of skeletal atoms;
    b. ascending enumeration pattern, which assigns the lower number on the occasion of the first difference to the
        (1) carbon atom of the saturated hydrocarbon state of the path which bears the greater number of hydrogen atoms;
        (2) heavier skeletal atom;
        (3) skeletal atom to which is bonded the
            (a) greater number of functional substituents;
            (b) heavier functional substituent;
            (c) more unsaturated skeletal bond.

EXAMPLE:

(1)



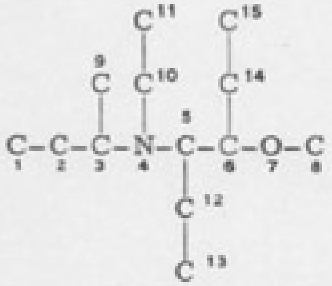
The enumeration proceeds from 5 to 6 according to 2a; from 6 to 7 according to 2b(1).

3. Continue to enumerate in the branching directions encountered according to the above procedure until a second terminal carbon atom is enumerated, thus establishing a main path-molecular main path-through the molecule. All unenumerated skeletal paths which have been by-passed during the establishment of the main chain are substituents thereof. See Ex. (2).
4. Enumerate, in the same ascending sequence and in the direction which leads away from the main path, the substituent skeletal paths in the ascending numerical order of their respective parent atoms and any branches of such paths in the same order described by rule 2 above for the first pass through. Each successive enumeration of a terminal carbon atom of a substituent path establishes a substituent main path. See Ex. (3).
5. Enumerate all unenumerated skeletal groups bonded to each successively established substituent main path in the same order described by rule 4 above for skeletal groups attached to the original, or molecular, main path before proceeding to the next higher numbered atom of the path which contains the parent atom of the substituent main path concerned.

The effect of the described procedure is the exhaustive enumeration of each skeletal substituent before the enumeration of any atom of a skeletal substituent which is attached to a higher numbered atom of the same parent path. When enumerated according to the above described procedure the molecular main path, and each substituent main path, will be recognizable as having an unbroken ascending numerical sequence; the parent atom of each substituent path will be recognizable as that enumerated atom to which such path is attached which breaks the descending numerical sequence of the substituent path.

EXAMPLE:

(2)

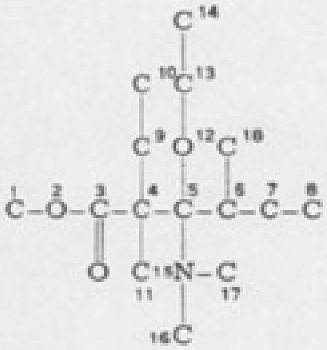


In the above formula atoms 1-8 is the molecular main path. Atoms 3, 4, 5, and 6 are the parent atoms of substituent paths 9, 10-11, 12-13, and 14-15, respectively.

6. Whenever a plurality of substituent skeletal paths are bonded to the same parent atom, enumerate such substituents as branching paths in the order described by rule 2 above.

EXAMPLE:

(3)



In the above formula note that the ethyl substituent 9-10 is enumerated before the methyl substituent 11 and that the propyl substituent, i.e. saturated hydrocarbon state of propoxy, is enumerated before the isopropyl group, saturated hydrocarbon state of dimethylamino.

3.2 CORRECT STARTING ATOM

Select as starting atom for the enumeration that terminal carbon atom which generates, according to the enumerating procedure described in Section 3.1, the enumeration pattern which assigns the lower number on the occasion of the first difference to the following features listed in their order of decreasing priority:

1. carbon atom to which is bonded the greater number of hydrogen atoms in the saturated hydrocarbon state of the molecule;
2. heavier skeletal atom;
3. skeletal atom to which is bonded the
   a. greater number of functional substituents;
   b. heavier functional substituent, considered one by one in ciphering order in the event of a plurality;
   c. more unsaturated skeletal bond.

Before evaluating feature 1. convert the molecule to the extent necessary, to the saturated hydrocarbon by executing the following operations:

1. Replace all hetero atoms which interrupt a carbon chain by carbon atoms on a one for one basis.
2. Replace all functional substituents by the number of hydrogen atoms (implied) equal to the valence thereof.
3. Saturate all multiple bonds of the residual structure by hydrogen atoms (implied).

In the event feature 1, above, is indecisive revive the formula to its fully derived state and test the remaining features in order.

In practice it is normally unnecessary to generate a complete enumeration pattern from each terminal carbon atom before making a decision, since the correct starting atom is usually apparent after competitive enumeration of the first few potential main path positions.

When two or more terminal carbon atoms generate enumeration patterns which cannot be distinguished by the selection criteria, such patterns are equivalent and any one is correct and will all yield the same cipher, unless a difference is established by stereoisomeric relationships as described in Section 8.

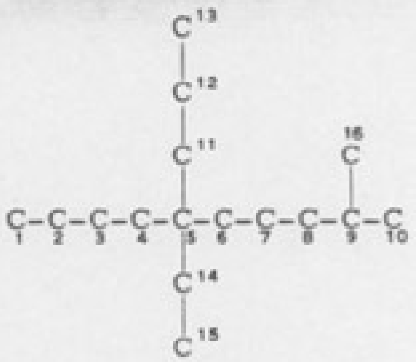
If the acyclic molecule is unbranched only criteria 2. and 3. apply.

3.3 SATURATED HYDROCARBONS

The correct starting atom is that terminal carbon atom which generates, in the manner described, the enumeration pattern which assigns the lower number on the occasion of the first difference to that carbon atom which bears the greater number of hydrogen atoms (implied). In case of a tie any one of the terminal carbon atoms which establish the tie may start the enumeration.

EXAMPLES:

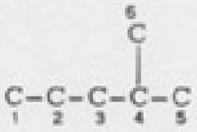
(1)



C4C(C3)EC3T

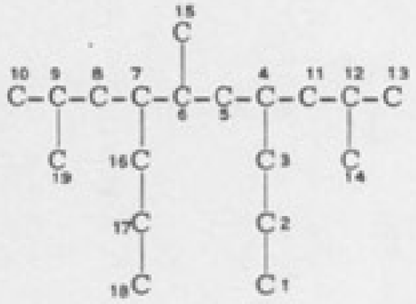
The lowest numbered path of unbroken ascending numerical sequence is the molecular main path, which may serve as a convenient basis for indexing, and nomenclature. Each branch whose lowest numbered atom exceeds by two or more the numerical value of the atom to which such branch is attached, thus breaking the ascending numerical sequence, is a substituent of the latter atom.

(2)



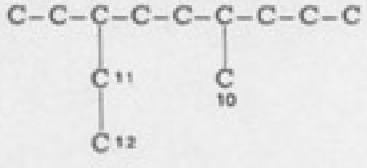
C3T

(3)



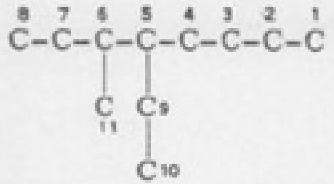
C3$\overset{4}{C}$(CT)C$\overset{6}{C}$M$\overset{7}{C}$(C3)CT

(4)



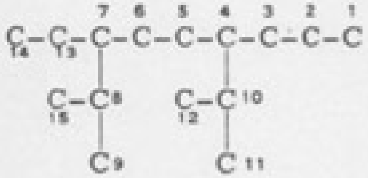
C3CMCCCE2

(5)



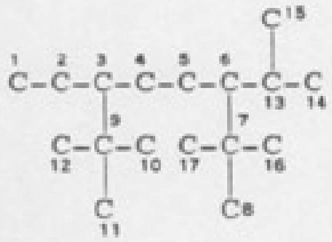
C4$\overset{5}{C}$E$\overset{6}{C}$ME

(6)



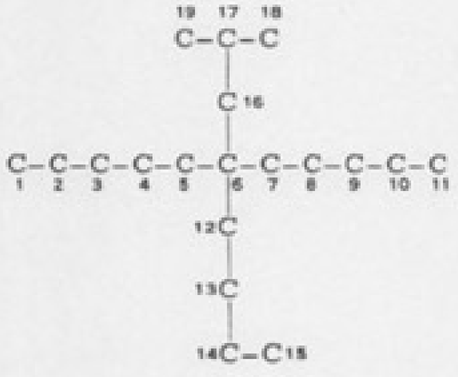
C3$\overset{4}{C}$TCC$\overset{7}{C}$ET

(7)

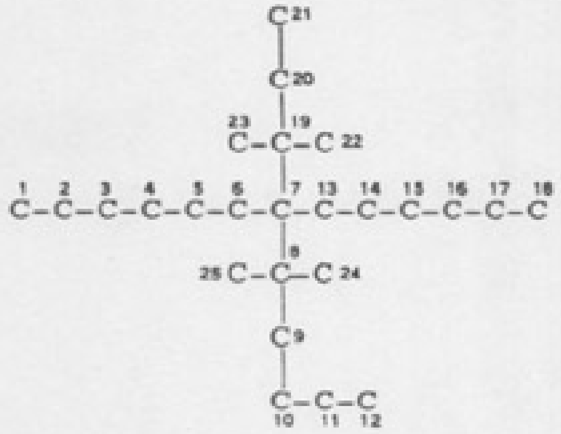


E$\overset{3}{C}$(CM3)$\overset{4}{C}$C$\overset{6}{C}$T$\overset{7}{C}$M3

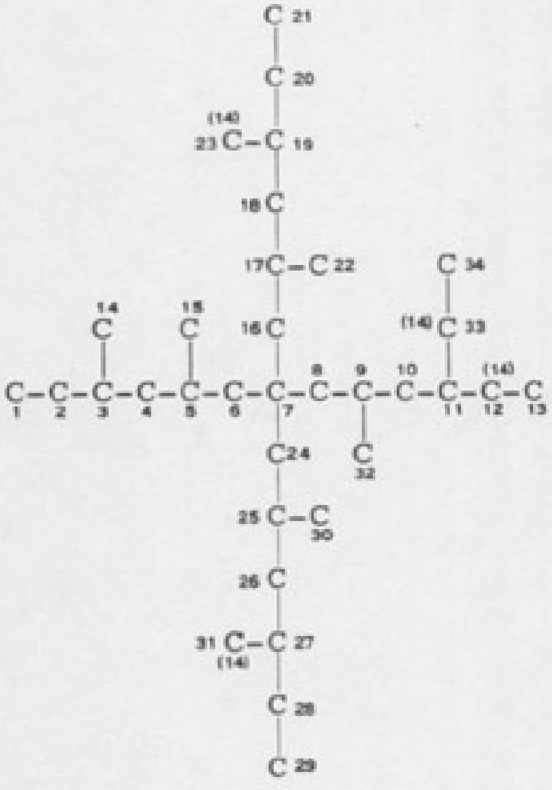
(8)



C5C(C4)(CT)C5

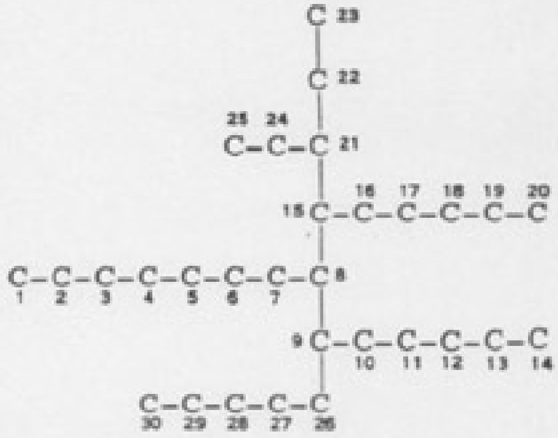
(9)


$\overset{7}{\mathrm{C}}\mathrm{(C6)2(}\overset{19}{\mathrm{C}}\mathrm{M2E)}\overset{8}{\mathrm{C}}\mathrm{M2C4}$ See 2.83

(10)


$\overset{7}{\mathrm{C}}\mathrm{(CCMCCME)3}\overset{8}{\mathrm{C}}\mathrm{CMC}\overset{11}{\mathrm{C}}\mathrm{E2}$

In the above formula atoms 1, 21, and 29 are equivalent starting atoms which win out over the closest contenders, atoms 13 and 34 at corresponding positions "14", as indicated by "(14)".

(11)


$\mathrm{C7}\overset{8}{\mathrm{C}}\mathrm{(}\overset{15}{\mathrm{C}}\mathrm{(CE2)C5)}\overset{9}{\mathrm{C}}\mathrm{(C5)2}$ See 2.83

(12)


M

(13)


E

(14)


T

(13)


C4

(14)


C7

The above described enumeration procedure for saturated hydrocarbons requires the ascending enumeration, as already set forth (section 2.3), always to pursue that branching direction which is richer in carbon, and in the event of a tie on carbon content, that branching path which becomes first richer in directly bonded hydrogen, i.e., the path whose ascending enumeration pattern from the branching point concerned assigns the lower number to the carbon atom which bears the greater number of hydrogen atoms at the first difference.

3.4 NAMING AND INDEXING OF ACYCLIC SATURATED HYDROCARBONS AS A SYSTEM OF STRAIGHT CHAINS

The enumeration patterns which are generated according to the procedure of this notation enable acyclic parent hydrocarbons to be named and indexed as a system of straight chains as illustrated by the following names and indexes for structures 1-11 above, in which the chains are cited in the order of decreasing chain length, only the first occurring of a given length being cited by name the remainder by locant:

(1) decane.propyl-5;ethyl-5;methyl-9.
C10.C3-5;C2-5;C-9.

(2) pentane.methyl-4
C5.C-4.

(3) decane.propyl-4,7;methyl-6,9,12.
C10.C3-4,7;C-6,9,12.

(4) nonane.ethyl-7;methyl-4.
C9.C2-7;C-4.

(5) octane.ethyl-5;methyl-6.
C8.C2-5;C-6.

(6) nonane.ethyl-4,7;methyl-8,10..
C8.C2-4,7;C-8,10.

(7) octane.ethyl-3,6;methyl-7,7,9.
C8.C2-3,6;C-7,7,9.

(8) undecane.butyl-6,propyl-6;methyl-17
C11.C4-6,C3-6;C-17.

(9) dodecane.hexyl-7;propyl-7;methyl8,8,19,19,
C12.C6-7;C3-7;C-8,8,19,19.

(10) tridecane.hexyl-7,7;ethyl-11;methyl-3,5,9,17,19,25,27.
C13.C6-7,7;C2-11;C-3,5,9,17,19,25,27..

(11) tetradecane.hexyl-8;pentyl-9;propyl-15;ethyl-21.
C14.C6-8;C5-9;C3-15;C2-21.

A structure can be reconstituted from its name by constructing and enumerating the main path and then proceeding to construct and enumerate each successive substituent chain to exhaustion before proceeding to the next main path substituent.

3.5 UNSATURATED HYDROCARBONS

Skeletal bonds are bonds which connect skeletal atoms, as stated in section 1. An acyclic skeletal bond is assigned the same number as the lower numbered atom to which it is attached. A skeletal bond is always the last configuration ciphered before ciphering of the higher numbered atom to which is is connected. A <u>triple bond</u> is ciphered by the division sign "÷"; a double bond, by the equality sign "=".

EXAMPLES: (cipher appears below compound):

(

(1) $\overset{6}{C}-\overset{5}{C}-\overset{4}{C}-\overset{3}{C}=\overset{2}{C}-\overset{1}{C}$

MC=CC3

(2) $\overset{6}{C}-\overset{5}{C}=\overset{4}{C}-\overset{3}{C}-\overset{2}{C}=\overset{1}{C}$

C=CCC=CM

(3) $\overset{1}{C}=\overset{2}{C}$

C=C

(4) $\overset{1}{C}=\overset{2}{C}=\overset{3}{C}$

C=C=C

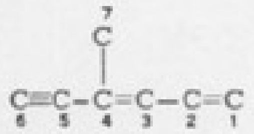
(5) $\overset{1}{C}\equiv\overset{2}{C}$

C÷C

(6) $\overset{1}{C}\equiv\overset{2}{C}-\overset{3}{C}\equiv\overset{4}{C}$

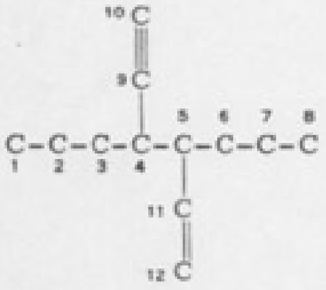
C÷CC÷C

(7)



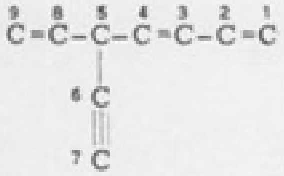
$C{=}CC{=}\overset{4}{C}MC{\div}C$

(8)



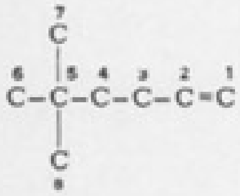
$C3\overset{4}{C}(C{\div}C)\overset{5}{C}(C{=}C)C3$

(9)



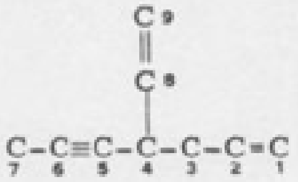
$C{=}C\overset{3}{C}{=}\overset{5}{C}C(C{=}C)C{\div}C$

(10)



$C{=}\overset{2}{C}CC\overset{5}{C}M3$

(11)



$\text{C=CC}\overset{4}{\text{C}}\text{(C=C)C+CM}$

3.6 DERIVATIVES CONTAINING FUNCTIONAL SUBSTITUENTS

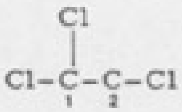
Hydrogen atoms bonded to carbon are not considered as substituents but as an integral part of the hydrpcarbon skeleton. Any hydrogen atom which is bonded to a skeletal hetero atom is a functional substituent of the hetero atom to which it is bonded. In the following formula the hydrogen atom attached to nitrogen is a functional substituent:

$$C-C-\overset{H}{N}-C$$

Any group which contains a carbon atom is not a functional substituent but contains part of the skeleton.

EXAMPLES:

(1)

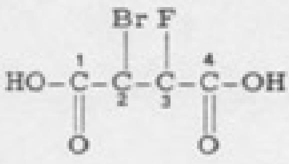


CK2CK

(2) $\overset{2}{C}-\overset{1}{C}-Cl$

EK

(3)

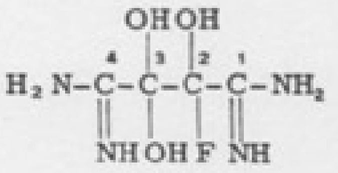


CVQCBCFCVQ

(4)

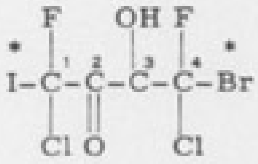
$\text{CVQ}\overset{2}{\text{C}}\text{F2}\overset{3}{\text{C}}\text{BCVQ}$

(5)



$\text{C(=NH)Z}\overset{2}{\text{C}}\text{QF}\overset{3}{\text{C}}\text{Q2C(=NH)Z}$

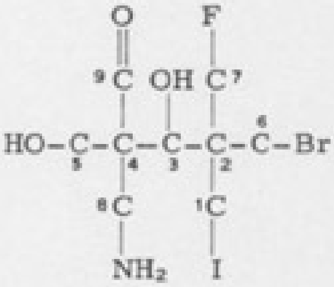
(6)



$\text{CF}\overset{*}{\text{K}}\text{ICV}\overset{3}{\text{C}}\text{Q}\overset{4}{\text{C}}\text{FK}\overset{*}{\text{B}}$

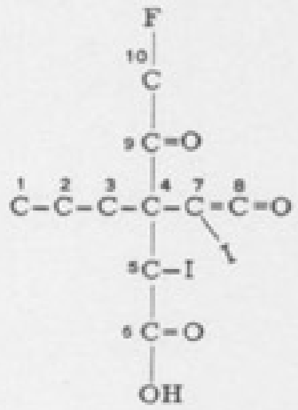
* decisive substituents

(7)



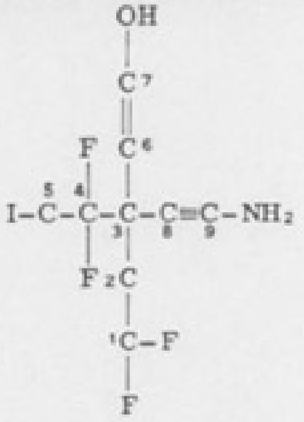
$\text{CI}\overset{2}{\text{C}}\text{(CB)(CF)}\overset{3}{\text{C}}\text{Q}\overset{4}{\text{C}}\text{(CZ)(CV)}\overset{5}{\text{C}}\text{Q}$

(8)



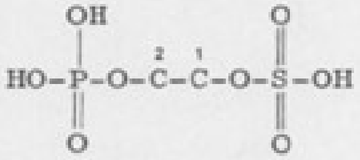
$\text{C3}\overset{4}{\text{C}}\text{(CI CV)(CVCF)}\overset{5}{\text{C}}\text{I}\overset{6}{\text{C}}\text{VQ}$

(9)



$\mathrm{CF2C\overset{3}{C}(\overset{6}{C}{-}CQ)(\overset{8}{C}{+}CZ)\overset{4}{C}F2CI}$

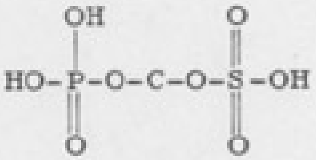
(10)



$$\mathrm{HO{-}\overset{OH}{\underset{O}{P}}{-}O{-}\overset{2}{C}{-}\overset{1}{C}{-}O{-}\overset{O}{\underset{O}{S}}{-}OH}$$

C(OSWQ)C(OPVQ2)*

(11)

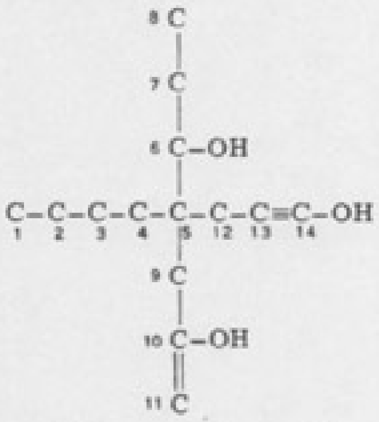


$$\mathrm{HO{-}\overset{OH}{\underset{O}{P}}{-}O{-}C{-}O{-}\overset{O}{\underset{O}{S}}{-}OH}$$

C(OPVQ2)(OSWQ)*

*Note. Atomic Weights are not rounded off, but fractional values are ignored unless decisive. In the preceding formula the phosphate radical is ciphered first since it is lighter in weight (4×16+31.975+2= 96.975) than the sulfate substituent weighing 97.066. In practice atoms common to both substituents, i.e. the four oxygen atoms and and one hydrogen atom, would be cancelled out and the aggregate weights of the residual atoms of the two substituents compared and resolved as PH (31.975) versus S (32.066).

(12)



$\mathrm{C4\overset{5}{C}(C\overset{9}{C}Q{=}C)(C\overset{12}{C}{+}CQ)\overset{6}{C}QE}$

3.61 FUNCTIONAL SUBSTITUENTS WHICH HAVE THE SAME WEIGHT BUT DIFFERENT CONFIGURATIONS

The following rule applies to situations wherein substituents of the above described types are bonded to

A. corresponding skeletal atoms whose paths are competing for prior enumeration,
B. the same skeletal atom so that the described substituents compete for prior ciphering.

RULE:

When functional substituents have the same weight but different configurations, that one is declared heavier which generates from the skeletal atom to which bonded into the body of the substituent the

(1) first heavier substituent atom, or the
(2) first more unsaturated substituent bond,

whichever occurs earlier, according to the generating procedure described in Section 3.62 below. In making this determination only correspondingly generated atoms and correspondingly generated bonds are compared, i.e. the first generated bond of substituent A with the first of substituent B, etc.; the first generated atom of substituent A with the first generated atom of substituent B; the second of A, with the second of B, etc., until either one generated atom is heavier than the corresponding atom(s) with which compared or one generated bond is more unsaturated than the corresponding bond(s) with which compared. The <u>first difference</u> which occurs forms the basis of the decision.

In the following examples the alphabetical order of the lower case letters indicates the order of bond generation; the numerals, the ascending numerical order of atom generation:

EXAMPLES:

(1)

$$\mathrm{O{=}N{-}O{-}C{-}\overset{O}{N}{=}O}$$

generating order of (O=N-O): $\mathrm{(C)\overset{a}{-}\underset{1}{O}\overset{b}{-}\underset{2}{N}\overset{c}{=}\underset{3}{O}}$

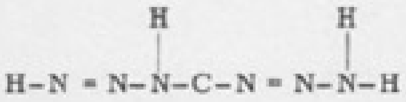
generating order of (NO_2): $\mathrm{(C)\overset{a}{-}\underset{1}{N}\overset{b}{-}\underset{2}{O}\overset{c}{=}\underset{3}{O}}$

The nitrite (–O–N=O) substituent generates the first heavier atom, oxygen "1", and is therefore declared heavier and ciphered after the contending nitro (NO_2) substituent whose correspondingly generated atom is nitrogen "1".

cipher: C(NW)(ONV)

NOTE: Throughout this notation system the bond connecting an oxygen atom directly and solely to another atom is represented by a double bond in the generation procedure thus signifying that the bond configurations of the two oxygen atoms bonded solely to the same other atom as in $-NO_2$ and $-SO_2OH$ are indistinguishable.

(2)



$$H-N=N-\overset{\overset{H}{|}}{N}-C-N=N-\overset{\overset{H}{|}}{N}-H$$

generating order of ($N=NNH_2$): (C) $\overset{a}{-}\underset{1}{N}\overset{b}{=}\underset{2}{N}\overset{c}{-}\underset{3}{N}\overset{d}{-}\underset{4}{H}\overset{e}{-}\underset{5}{H}$

generating order of ($NHN=NH$): (C) $\overset{a}{-}\underset{1}{N}\overset{b}{-}\underset{2}{H}\overset{c}{-}\underset{3}{N}\overset{d}{=}\underset{4}{N}\overset{e}{-}\underset{5}{H}$

The letters and numbers indicate correspondence as stated above. In this example the corresponding "a" bonds and "1" atoms are identical. The first difference occurs upon generation of the corresponding "b" bonds. The "b" bond of the ($N=NH_2$) substituent is the more unsaturated so that the substituent ($N=NNH_2$) containing it is declared heavier and ciphered last.

cipher: C(NHN=NH(N NZ))

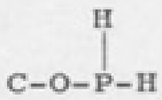
3.62 ORDER OF GENERATING AND CIPHERING SUBSTITUENT ATOMS AND BONDS. PARENTHESES

When a plurality of substituent groups is attached to the same previously generated substituent atom, cipher such groups in the same order and manner in which they would be ciphered if such groups were functional substituents of the same skeletal atom.

The atoms and bonds which constitute a functional substituent are generated according to the following rules:

1. The first atom of a substituent to be generated is that substituent atom which is directly bonded to the skeletal atom. This first generated substituent atom, and each successive substituent atom as generated, becomes the latest generated substituent atom, which is referred to in the following rules for generating substituent atoms further removed from the skeletal atom.

EXAMPLE:



$$C-O-\overset{\overset{H}{|}}{P}-H$$

The oxygen atom is generated first.

2. A substituent bond is generated (and ciphered—if multiple) immediately before the next atom to be generated to which the bond is attached.

EXAMPLES:

(2) $C=\overset{1}{N}-\overset{2}{H}$

generating order: C = NH

cipher: C(=NH)

(3) C–N = N–H

generating order: $C\overset{1}{N}\overset{2}{=}\overset{3}{N}\overset{4}{H}$ See rule 3.

cipher: O(N = NH)

Note. Single bonds are not expressed but implied in the generating order and cipher.

3. When only one ungenerated group is bonded to the latest generated substituent atom, that ungenerated atom which is directly bonded to the latest generated atom is next generated.

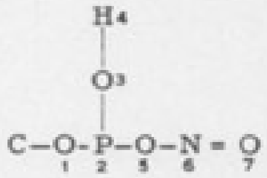
EXAMPLES:	CIPHERS:
(4) $C-\overset{1}{O}-\overset{2}{N}=\overset{3}{O}$	C(ONV)
(5) $C-\overset{1}{N}=\overset{2}{N}-\overset{3}{N}=\overset{4}{N}H$	C(N = NN = NH)
(6) $C-\overset{1}{S}-\overset{2}{S}-\overset{3}{H}$	C(SSH)

The ascending numerical order shown indicates the sequence in which the atoms are generated (and ciphered).

4. When two or more ungenerated groups of different weights are bonded to the latest generated substituent atom, such groups are generated (and ciphered) in the order of their increasing weights.

EXAMPLES:

(7)

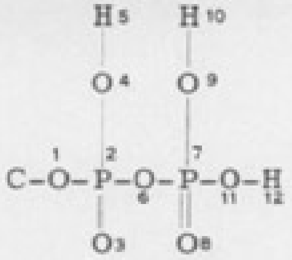


$$C-\underset{1}{O}-\underset{2}{\overset{\overset{\overset{H_4}{|}}{O_3}}{\overset{|}{P}}}-\underset{5}{O}-\underset{6}{N}=\underset{7}{O}$$

generating order $C\overset{1}{O}\overset{2}{P}\overset{3}{O}\overset{4}{H}\overset{5}{O}\overset{6}{N}=\overset{7}{O}$

cipher: C(OPQ(ONV))

(8)



$$\mathrm{C\overset{1}{-}O-\overset{2}{P}(-O^{3})(-O^{4}-H^{5})-\underset{6}{O}-\overset{7}{P}(=O^{8})(-O^{9}-H^{10})-\underset{11}{O}-\underset{12}{H}}$$

generating order: $\mathrm{C\overset{1}{O}\overset{2}{P} = \overset{3}{O}\overset{4}{O}\overset{5}{H}\overset{6}{O}\overset{7}{P} = \overset{8}{O}\overset{9}{O}\ \overset{10}{H}\ \overset{11}{O}\ \overset{12}{H}}$

cipher: C(OPVQOPVQ2)

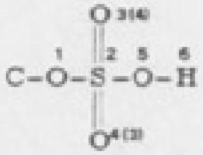
(9)

$$\mathrm{C-\overset{1}{O}-\overset{2}{S}(=O^{3})-\overset{4}{O}-\overset{5}{H}}$$

generating order: $\mathrm{C(\overset{1}{O}\overset{2}{S} = \overset{3}{O}\overset{4}{O}\overset{5}{H})}$

cipher: C(OSVQ)

(10)



$$\mathrm{C-\overset{1}{O}-\overset{2}{S}(=O^{3(4)})(=O^{4(3)})-\overset{5}{O}-\overset{6}{H}}$$

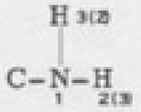
generating order: $\mathrm{C\overset{1}{O}\overset{?}{S} = \overset{3}{O} = \overset{4}{O}\overset{5}{O}\overset{6}{H}}$

cipher: C(OSWQ)

5. When a plurality of identical ungenerated groups is bonded to the latest generated substituent atom, such groups may be generated (and ciphered) in any order with respect to one another.

EXAMPLES:

(11)

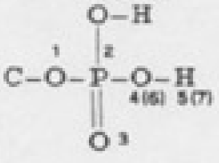


$$\mathrm{C-\underset{1}{N}(-H^{3(2)})-\underset{2(3)}{H}}$$

generating order: CNHH

cipher: CZ

(12)



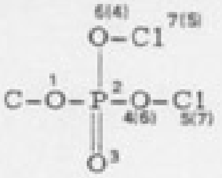
$$\mathrm{C-\overset{1}{O}-\overset{2}{P}(=O^{3})(-\overset{6(4)}{O}-\overset{7(5)}{H})-\underset{4(6)}{O}-\underset{5(7)}{H}}$$

g

generating order: $\mathrm{C\overset{1}{O}\overset{2}{P} = \overset{3}{O}\overset{4}{O}\overset{5}{H}\overset{6}{O}\overset{7}{H}}$

cipher: C(OPVQ2)

(13)

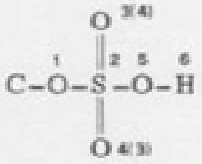


$$\mathrm{C-\overset{1}{O}-\overset{2}{P}(=O^{3})(-\overset{6(4)}{O}-\overset{7(5)}{Cl})-\underset{4(6)}{O}-\underset{5(7)}{Cl}}$$

generating order: $\mathrm{C\overset{1}{O}\overset{2}{P} = \overset{3}{O}\overset{4}{O}\overset{5}{Cl}\ \overset{6}{O}\ \overset{7}{Cl}}$

cipher: C(OPV(OK)2)

(14)

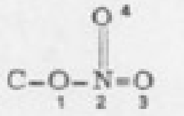


$$\mathrm{C-\overset{1}{O}-\overset{2}{S}(=O^{3(4)})(=O^{4(3)})-\overset{5}{O}-\overset{6}{H}}$$

generating order: $\mathrm{C\overset{1}{O}\overset{2}{S} = \overset{3}{O} = \overset{4}{O}\overset{5}{O}\overset{6}{H}}$

cipher: C(OSWQ)

(15)



$$\mathrm{C-\underset{1}{O}-\underset{2}{N}(=O^{4})=\underset{3}{O}}$$

generating order: $\mathrm{C\overset{1}{O}\overset{2}{N}=\overset{3}{O}=\overset{4}{O}}$

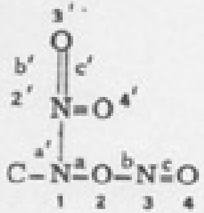
cipher: C(ONW)

6. When two or more substituent groups having the same weight but different configurations are bonded to the latest generated substituent atom, such groups are generated in the order in which there is generated from the latest generated atom into the contending groups (1) the first heavier atom or (2) the first more unsaturated bond whichever occurs earliest in the logical order in which the substituent atoms and bonds are generated, as set forth in rules 1-5 above. In this determination atoms and bonds are compared which occur in the same relative position in the sequential order in which they are generated in the respective substituent groups, i.e. first generated bond of one substituent group versus first generated bond of contending group, first atom versus first atom, etc.

In the following examples the lower case letters and their corresponding primes indicate correspondingly generated bonds; the numerals and their primes, correspondingly generated atoms. Groups are ciphered in the order of their increasing weights, as declared. See 3.61.

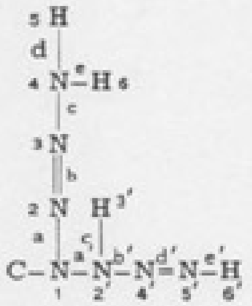
EXAMPLES:

(16)



cipher: C(N(NW)ONV)

(17)

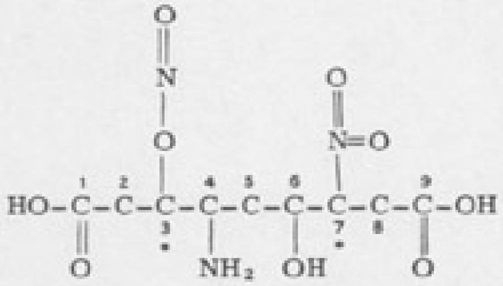


cipher: C(NN=NZ(NHN=NH))

The "b" bond is more unsaturated than the corresponding "b" prime bond so that the group containing the former is generated first.

3.63 Functional Substituents of Same Weight But Different Configurations As Decisive Factor in Determining the Order of Enumeration.

EXAMPLE:



CVQCC(ONV)CZCCQC(NW)CCVQ

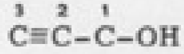
*decisive skeletal positions

3.64 Order of Enumeration with Respect to Functional Substituents and Skeletal Bonds.

When the order of enumeration is decided by the weight and/or distribution of a functional substituent, it remains unaffected by the distribution or degree of unsaturation of skeletal bonds, the latter feature being of lower priority as expressed in Section 1. and in the enumeration rules for acyclic molecules.

EXAMPLES:

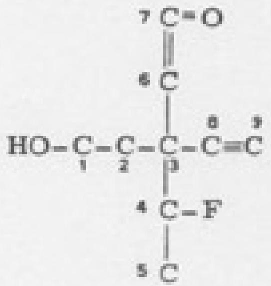
(1)



$\overset{3}{C}\equiv\overset{2}{C}-\overset{1}{C}-OH$

cipher: CQC+C

(2)



cipher: $CQC\overset{3}{C}(C=CV)(C+C)\overset{4}{C}FM$

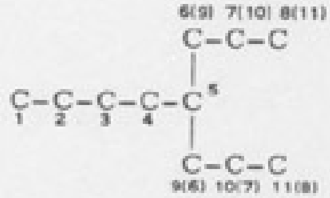
3.7 DERIVATIVES HAVING HETEROGENEOUS SKELETONS

The weight and distribution of hetero atoms which interrupt a carbon chain are given higher priority in the determination of the order of enumeration than are hetero atoms which comprise functional substituents, as set forth in Section 1. and incorporated in the enumeration rules for acyclic molecules. When the order of enumeration is decided by a skeletal hetero atom, it remains unaffected by the nature or distribution of functional substituents.

In the following examples note that the enumeration pattern of each hydrocarbon derivative is always congruent with that of the corresponding saturated parent hydrocarbon no matter what the nature or distribution of derived features may be.

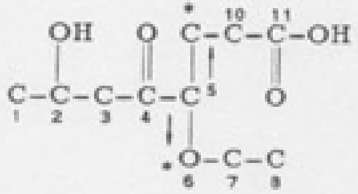
EXAMPLES:

(1)



The above numerals in parentheses indicate that either propyl path may be enumerated first.

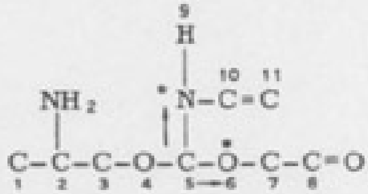
(2)



MCQCCVC(CCCVQ)OE

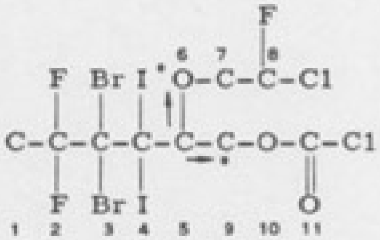
The asterisks indicate the decisively compared skeletal atoms; the arrows, the competing directions of ascending enumeration.

(3)



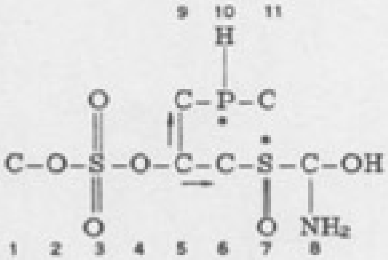
MCZCOC(NHC=C)OCCV

(4)



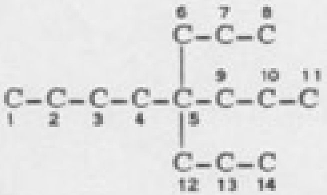
MCF2CB2CI2C(COCVK)OCCFK

(5)



MOSWOC(CPHM)CSVCZQ

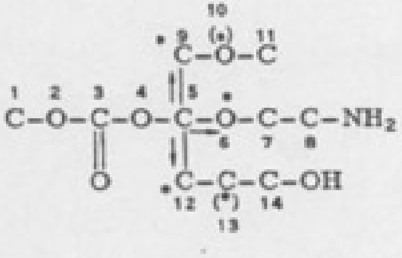
(6)



The three propyl branches may be enumerated in any order.

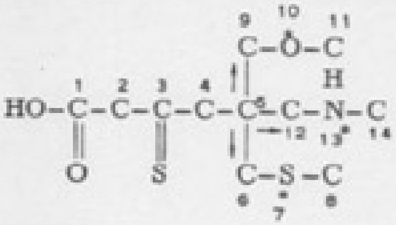
ECCC(CE)3

(7)



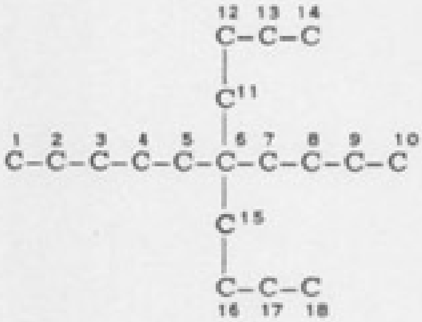
MOCVOC(COM)(CCCQ)OCCZ

(8)



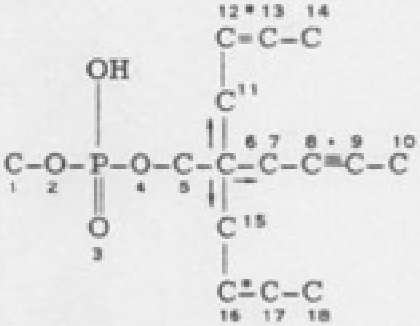
CVQCC(=S)CC(COM)(CNHM)CSM

(9)



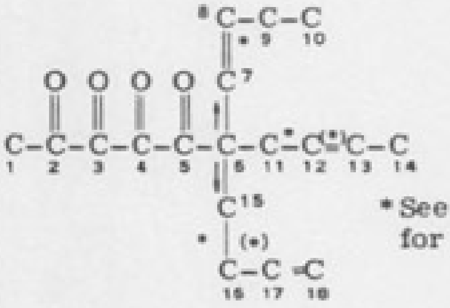
C5C(C4)3

(10)



MOPVQOCC(CC=CM)(C4)CC÷CM

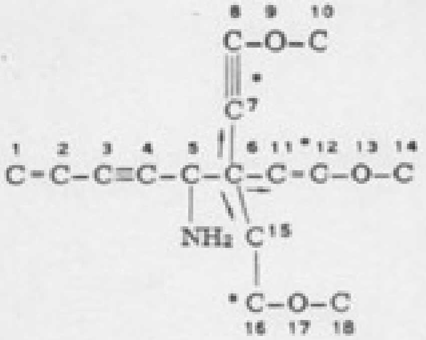
(11)



*See Table V for { }.

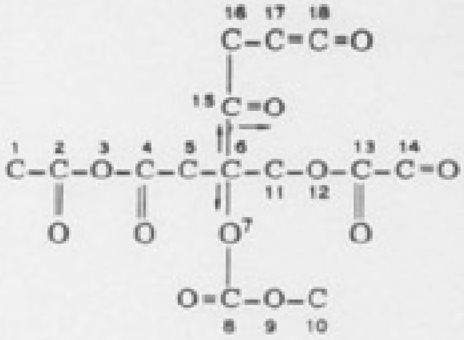
M*{CV}*4C(CC=CM)(CCC=C)C=CE

(12)



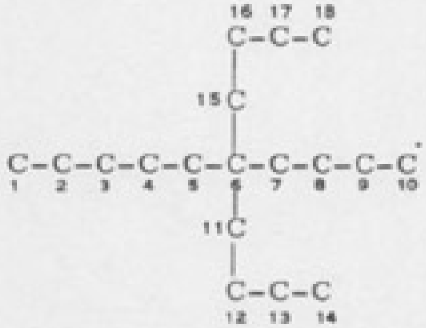
C=CC+CCZC(C=COM)(CCOM)C+COM

(14)

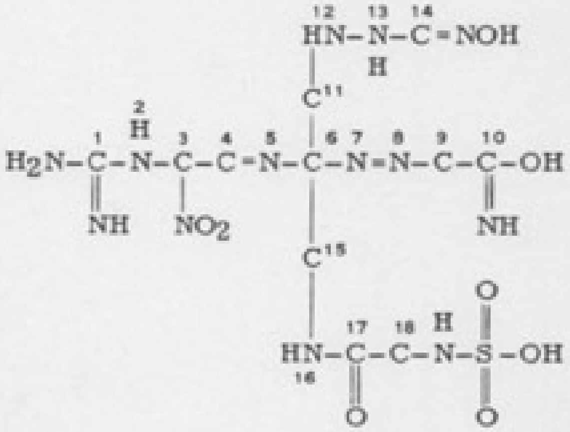


MCVOCVCC(COCVCV)(CVCC=CV)OCVOM

(13)



(15)



C(=NH)ZNHC(NW)C=NC(CNHNHC(NQ))
(CNHCVCNH(SWQ))N=NCC(=NH)Q

4.0 MONOCYCLIC COMPOUNDS

A monocyclic compound is a ring compound which can be converted to an open chain by the scission of a single ring bond. The fact that a string of atoms is hooked "head-to-tail" to form a closed path introduces an additional order of complexity beyond that exhibited by acyclic compounds and makes the selection of a starting point for an unambiguous enumeration more complicated. In monocyclic compounds, and in other ring compounds as well, not only must the ascending enumeration follow chain branches in a logical way but it must also choose between a clockwise and a counter-clockwise ring direction. It is convenient to visualize the ring as being a main chain and any skeletal substituents of the ring as substituents of the chain. The logical manner of enumerating acyclic ring substituents and acyclic chain substituents is identical.

4.1 GENERAL ORDER OF ASCENDING ENUMERATION

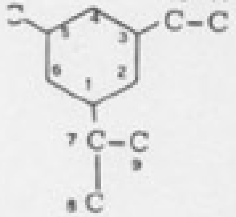
The ring atoms are enumerated first, serially around the ring. Next, any skeletal substituents attached to the ring are enumerated in the ascending numerical order of the ring atoms to which such substituents are attached. Skeletal substituents are enumerated as though branches of an open chain. When two skeletal substituents are attached to the same ring atom, that one is enumerated first which would be enumerated first if the two were unenumerated branches of the same chain atom (See Sec. 3.).

In the examples below the formulas are correctly enumerated. The procedure for selecting the correct starting atom and ring direction for the enumeration is set forth in the next section.

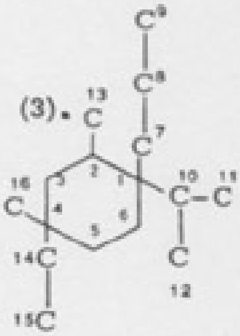
EXAMPLES:

(1)

(2)



(3).



4.2 CORRECT STARTING ATOM AND RING DIRECTION OF ASCENDING ENUMERATION

Begin the enumeration with that ring atom and continue to enumerate around the ring in that direction (clockwise or counter clockwise) which generates the order of ascending enumeration (enumeration pattern) which assigns the lower number on the occasion of the first difference to the following structural features listed in their order of decreasing priority:

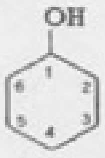
1. ring atom to which is bonded the
   a. greater number of skeletal substituents;
   b. skeletal substituent having the
      (1) greater number of skeletal atoms;
      (2) ascending enumeration pattern of the substituent in the saturated hydrocarbon state which assigns the lower number on the occasion of the first difference to that carbon atom which bears the greater number of hydrogen atoms;
2. features described by the updating rule (Sec. 2.61) in their same order of priority.

Only those potential starting atoms which tie on the basis of all features of higher priority may contend on the basis of the feature of next lower priority. Those contending atoms which fail to satisfy the condition just stated are eliminated from further contention.

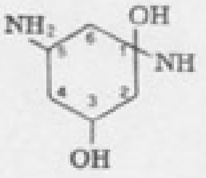
When a plurality of ring atoms and/or directions tie on the basis of all the listed features, begin the enumeration with any one of such atoms and/or directions.

In the determination of the "greater number of . . . substituents" it is critical to keep in mind that one is greater than zero, that is to say, an atom having one substituent has a greater number of substituents than one which has none. In formulas 1-4 below atoms "1" bear a greater number of substituents than any other atom of the ring concerned.

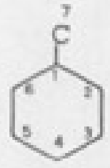
(1)



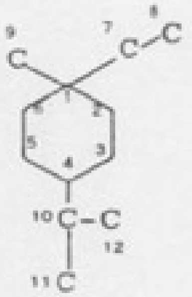
(2)



(3)



(4)

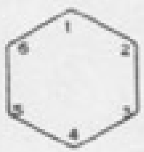


The enumeration of formulas 5-21, below, is determined solely by the updating rule:

(5)

3L3

(6)



6L6

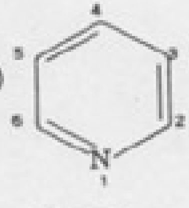
(7)

6R6

(8)

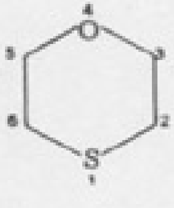
6n:LLL:LL

(9)



6nRR3R

(10)

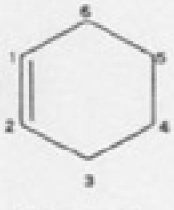


6SLLOLL

(11)

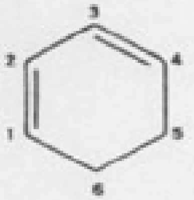
6nRnRRR

(12)



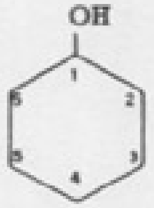
6L:LL4

(13)



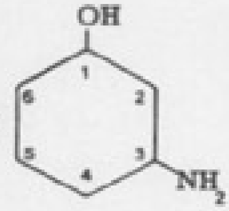
6L:LL:LLL

(14)



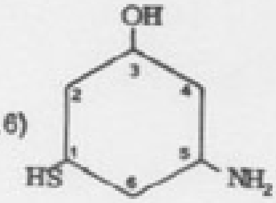
6LQL5

(15)



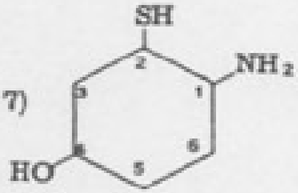
6LQLLZL3

(16)



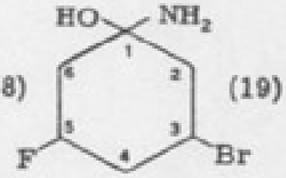
6L(SH)LLQLLZL

(17)



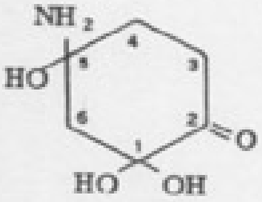
6LZL(SH)LLQLL

(18)



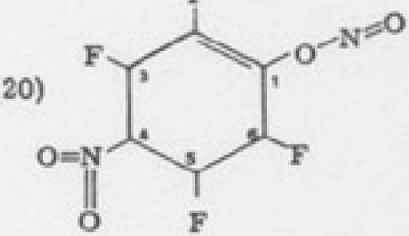
6LZQLLBLLFL

(19)



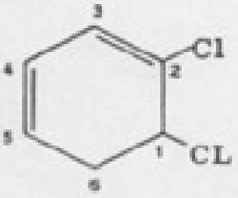
6LQZLVLLLZQL

(20)



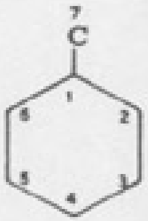
6L(ONV):LFLFL(NW)LFLF

(21)



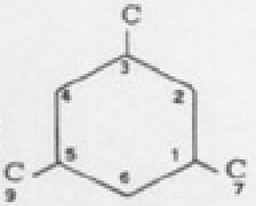
6LKLK:LL:LL

(22)



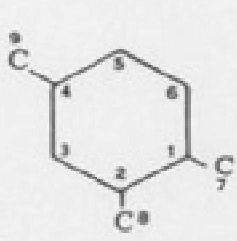
6LML5

(23)



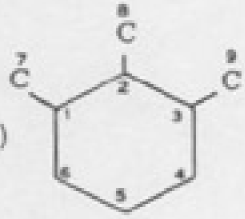
6LMLLMLLML

(24)



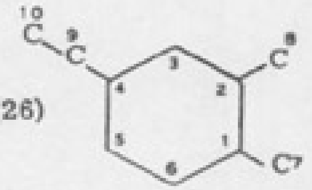
6LMLMLLMLL

(25)



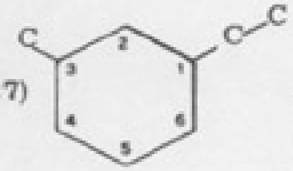
6LMLMLML3

(26)



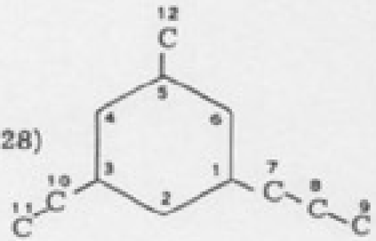
6LMLMLLELL

(27)



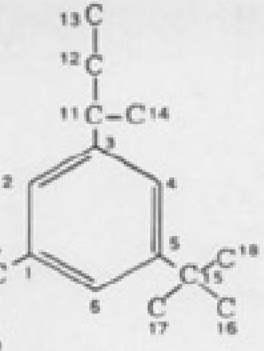
6LELLML3

(28)



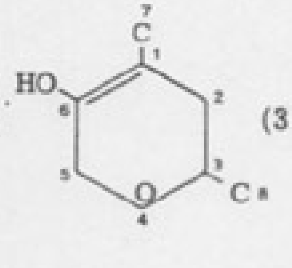
6L(C3)LLELLML

(29)



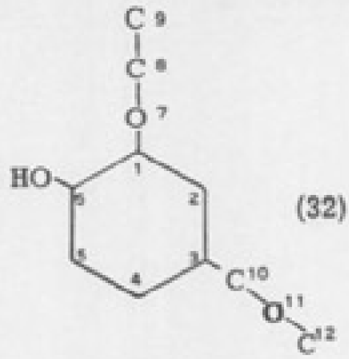
6R(CT)RR(CME)RR(CM3)R

(30)



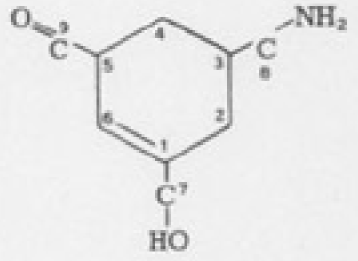
6LMLLMOLLQ:

(31)



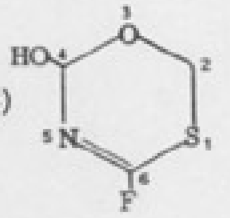
6L(OE)LL(COM)LLLQ

(32)



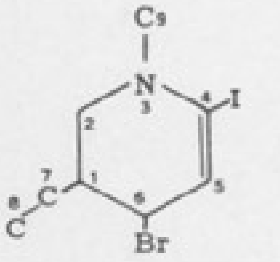
6L(CQ)LL(CZ)LL(CV)L:

(33)



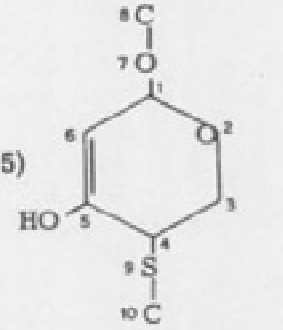
6SLOLQn:LF

(34)



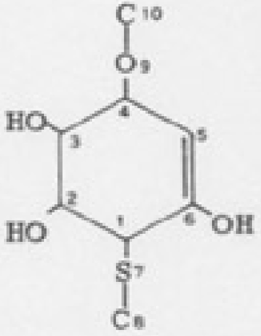
6LELnMLI:LLB

(35)



6L(OM)OLL(SM)LQ:L

(36)



6L(SM)LQLQL(OM)L:LQ

5.0 FUSED RING AGGREGATES. DEFINITION OF FUSION

Fused ring aggregates are compounds in which the rings are joined to one another solely by one and/or two atom interfaces, which are called fused faces.

When two rings are joined by a single atom, which atom is not common to a third ring, the rings are described as spiro-fused.

EXAMPLES:

*A and B are not spiro-fused, but each ortho-fused to rings "C".

When two rings are joined by an interface of two, and only two, atoms the rings are described as ortho-fused.

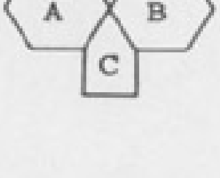
EXAMPLES:

(1)

(2)

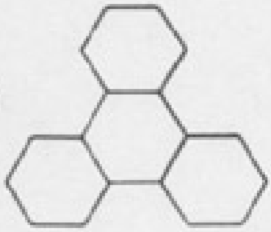
(4)

(3)



(5)

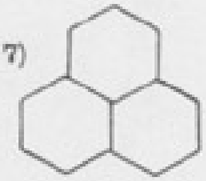
(6)



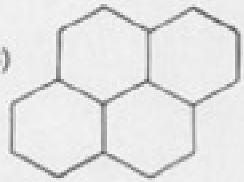
When a ring aggregate contains two rings joined by an interface of two atoms and at least one of such atoms if fused to a third ring, the rings involved are described as ortho-and peri-fused and the aggregate as condensed. Rings, A, B, and C of Sec. 5.0 are peripherally condensed. In this notation the term "ortho-fused" includes "ortho- and peri-fused".

EXAMPLES:

(7)



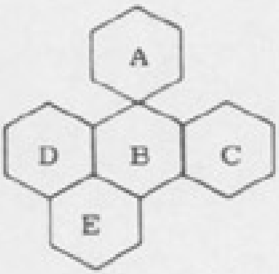
(8)



All three types of ring fusion described above may exist in the same ring aggregate.

EXAMPLE:

(9)



Rings A and B are spiro-fused, rings B and C are ortho-fused, and rings B, D, and E are ortho- and peri-fused.

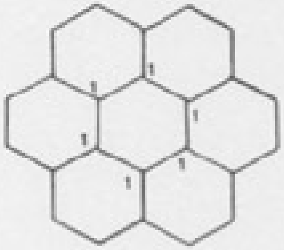
The only types of ring fusion recognized by the present scheme are the types described above. Ring interfaces of more than two atoms are characterized either as ring bridges, or as comprising the closed path which connects the component systems of a circular ring assembly.

5.01 Interior Fused Atoms of Condensed Ring Aggregates

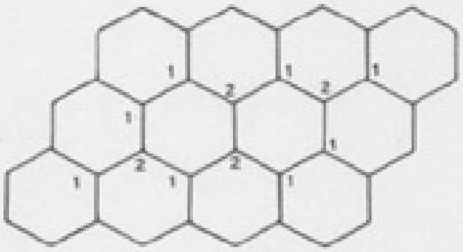
Interior fused atoms, normally, are either one or two bonds removed from the nearest peripheral atom and are common to at least three fused rings. These types of atoms are labelled by the figure "1", where one removed, and by the figure "2", where two bonds removed, from the nearest peripheral atom in the following formulas.

EXAMPLES:

(1)



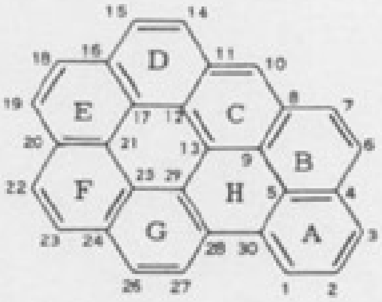
(2)



As is evident upon inspection of the above formulas the added structural feature of ring fusion further complicates the selection of a starting atom and an ordered direction of ascending enumeration. In monocyclic compounds, because of the single ring contained, no competition exists between different rings for prior enumeration as is the case with fused ring aggregates. In addition there exist in fused ring aggregate compounds branching ring paths as well as the possibility of branching chains. Still another obstacle to line formula notation is the "fickle" nature of the aromatic double bond, as represented in Kekule fashion, which permits such a bond to be drawn in a number of chemically equivalent but geometrically different positions of the planar fused ring system. The stated difficulties are overcome in the present system by (1) enumerating the rings sequentially in a constant peripheral direction from a starting point based on hydrogen distribution in the saturated hydrocarbon state of such rings, (2) using the R symbol so as to avoid localization of the aromatic "resonating" double bond, and (3) using the symbols "Y" and "y" to indicate the branching directions of the ring bonds which diverge from fused positions.

5.02 Geometric Significance of the Symbols "Y" and "y"

The symbols "Y" and "y" are used to represent ortho-fused carbon atoms as illustrated by the cipher of the formula below.



$6R3\overset{4}{Y}\overset{5}{y}RRY\overset{9}{y}R\overset{11}{Y}\overset{12}{y}\overset{13}{y}RR\overset{16}{Y}\overset{17}{y}RR\overset{20}{Y}\overset{21}{y}RR\overset{24}{Y}yRRY\overset{29}{y}Y$

The three prongs of the "Y" symbol are viewed as two arms and a leg which simulate the three bond directions which radiate from each fused position. The leg of the upper case letter "Y" is always that peripheral bond which extends from the Y atom (peripheral fused atom) in the peripheral direction which is opposite to that of ascending enumeration. The remaining two prongs of the Y are considered as arms which extend in the direction of ascending enumeration and embrace the next succeeding peripheral ring, if any. In the above cipher the leg of the Y which represents atom "8" simulates the bond connecting atoms "7" and "8"; the arms thereof simulate the bonds which connect atom "8" to atoms "9" and "10".

In like manner the lower case letter "y" simulates the three fused bonds which radiate from an interior fused atom. In the latter case the leg of the "y" is that bond which connects the "y" atom with the next lower numbered atom, e.g. the leg of the atom "13" y is the bond connecting atoms "12" and "13", the remaining two bonds are the arms.

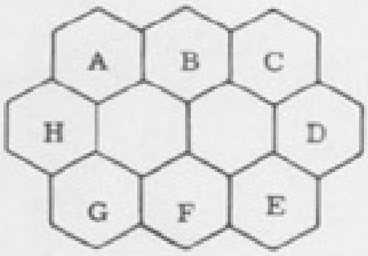
The Y and y symbols are indispensable to reconstruction of the formula from the cipher since the size of the ring embraced by the arms of each Y or y atom is expressed by a numerical suffix after the symbol concerned, if the size is other than six. Ring size six occurs at such high frequency in fused ring systems that size six is implied by the absence of a numerical suffix after the Y or y symbol involved. Since ring atoms are ciphered in the same order as enumerated, it is quite straightforward to reconstitute the ring system from the cipher by constructing each successive ring of the size and orientation indicated by each successive Y or y symbol as encountered in the cipher.

5.1 CONCEPT OF PERIPHERAL RINGS

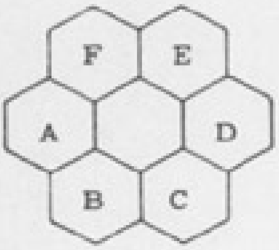
A fused ring system is considered to be made up of peripheral rings. A peripheral ring is a ring which contains at least one atom which lies on the periphery (outermost largest ring) of the ring system concerned. All of the fused ring systems illustrated above in Sec. 5.00 and 5.01 and, significantly, all of the fused ring systems reported in the Revised Ring Index (1960) are constituted wholly by peripheral rings, i.e. considering those rings which are represented by contiguous polygons in the reference plane (plane of paper).

In Ovalene (RRI 7653) and Coronene (RRI 7392,) the ten and seven ring systems, respectively, shown below, it is apparent that the peripheral rings, indicated by the capital letters, consume all of the ring atoms:

(1)



(2)

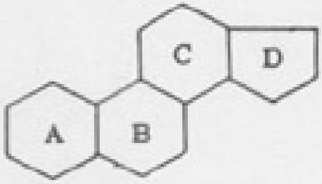


The concept of peripheral rings is basic to an understanding of the method of enumeration of fused ring systems which will be described in the next section. The order of ascending enumeration proceeds around the ring system peripheral ring by peripheral ring in sequence, as shown by the alphabetical order of the rings illustrated above.

The rings of a non-condensed, fused system (See Sec. 5.0) are peripheral to the maximum degree in that all atoms of the ring system are peripheral.

In such systems the peripheral atoms are enumerated in unbroken sequence since there are no interior atoms to interrupt their enumeration, as is the case in condensed systems. The rings of the steroid nucleus are enumerated in the alphabetical sequence indicated below:

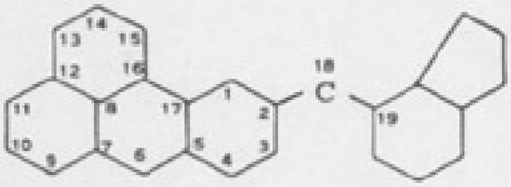
(3)



5.2 GENERAL ORDER OF ASCENDING ENUMERATION OF THE RING ATOMS OF A FUSED RING AGGREGATE.

This section describes only the atom by atom path which the ascending enumeration must follow when proceeding from any given peripheral atom in a given peripheral direction. The procedure for selecting the correct starting atom and peripheral direction for the enumeration of a particular fused ring system is described in the Section 5.3. The discussion of this section is pertinent not only to the enumeration of compounds classified as fused ring aggregates and bridged ring aggregates, which contain a single ring system, but also to the determination of the direction of enumeration around a substituent ring system of a ring assembly after the first atom of such system has been enumerated, as illustrated by atom "19" below:

(1)

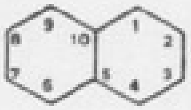


The path which the ascending enumeration of a fused ring system must follow is defined by the following rule:

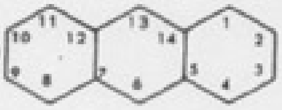
Proceeding from a given peripheral atom of a given peripheral ring and in a predetermined peripheral direction (clockwise or counterclockwise) enumerate serially all unenumerated atoms, which can be enumerated without partitioning the aggregate, of each successive peripheral ring until all atoms of the system have been enumerated.

EXAMPLES (See next section for selection of starting atom and direction):

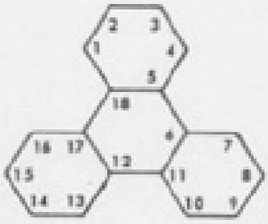
(2)



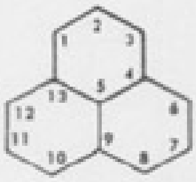
(3)



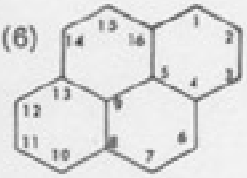
(4)



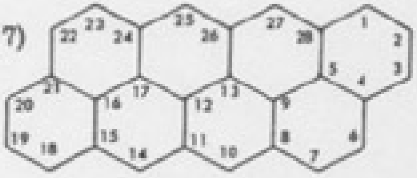
(5)



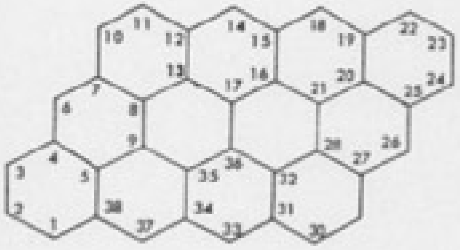
(6)



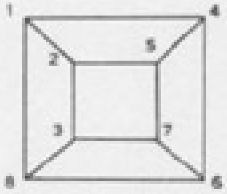
(7)



(8)



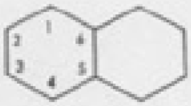
(9)



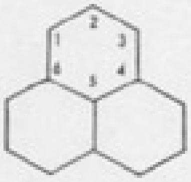
Note that in none of the above examples does the enumeration partition, or sever, the aggregate. The ring system is partitioned by the enumeration whenever in a given ring two peripheral atoms which are separated from each other by one or more interior bonds are enumerated in the same unbroken ascending sequence, as illustrated by the following examples:

INCORRECT ENUMERATION:

(10)



(11)



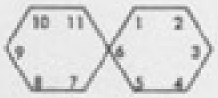
In case A the 5-6 sequence severs the aggregate; in case B, the 4-5-6 sequence.

5.21 Systems Containing Spiro-Fused Rings

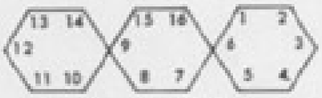
Spiro-fused atoms are enumerated when first encountered and skipped over when re-encountered by the ascending enumeration. Because of the requirement that the peripheral direction of enumeration be constant, figure-eight type of enumeration around spiro rings is forbidden.

EXAMPLES:

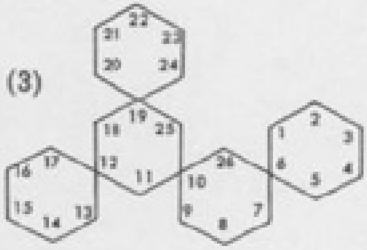
(1)



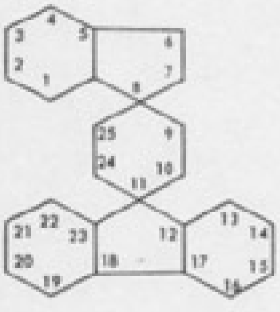
(2)



(3)

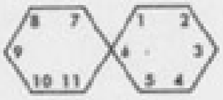


(4)



INCORRECT ENUMERATION:

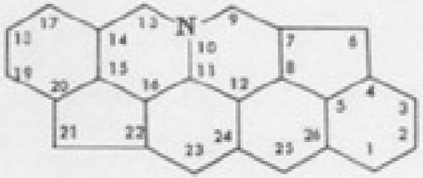
(5)



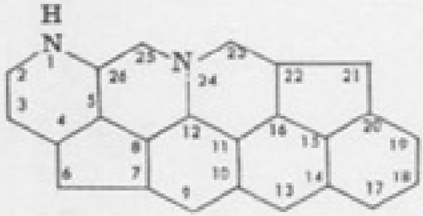
The following examples of correctly enumerated ring systems illustrate that the general order, or path direction, of ascending enumeration of ring positions does not change although the specific starting point and peripheral direction depends upon hydrogen distribution and, in symmetrical systems, upon the nature and distribution of skeletal substituents and derived features.

EXAMPLES:

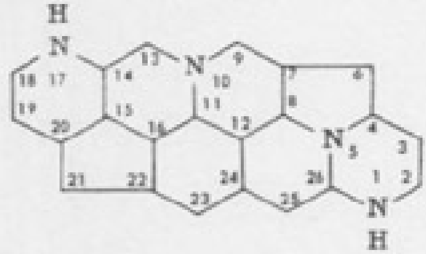
(6)



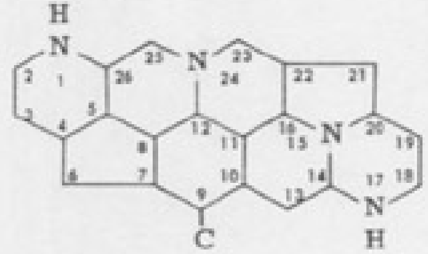
(7)



(8)



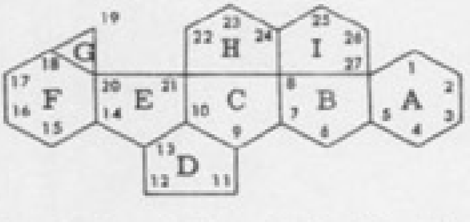
(9)



5.22 Systems Containing Peripheral Atom Common to Two Fused Faces and/or Interior Atom Common to Four Fused Faces

The first type of atom concerned is illustrated by atoms 20, 21, and 27 in the following ring system:

(1)



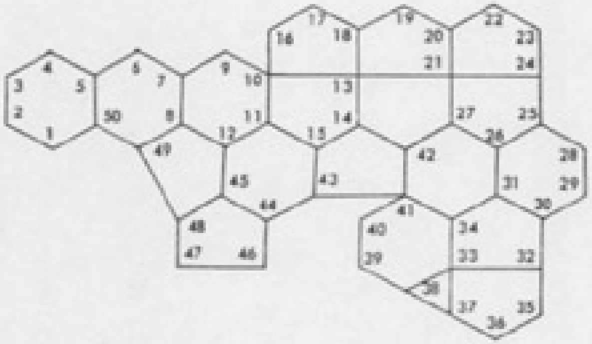
$6L4\overset{5}{Y}5L\overset{7}{Y}5\overset{8}{y}5,5\overset{9}{Y}5\overset{10}{y}5LL\overset{13}{Y}5\overset{14}{Y}L3\overset{18}{Y}3L\overset{20}{Y}6,5\overset{21}{Y}5,$
5LLY5LLY5,6

As already set forth (Sec. 5.0), atoms of the subject type are not characterized as spiro in the present notation. Atoms 20, 21, and 27 above present no problem for enumeration since all of the interior atoms, if any (atom 8) of the two rings to which each of such atoms is common have been subject to prior enumeration. In cases wherein both of the interior bonds connected to the peripheral atom lead to one or more unenumerated interior atoms a rule is required by which an unambiguous order of enumeration may be assigned to such unenumerated atoms. In all such cases the following rule applies:

Whenever there is enumerated a peripheral atom to which two unenumerated interior atoms are bonded, as illustrated by the formula below, enumerate first that one of such atoms which occurs in the ring which contains the peripheral bond which connects the two latest enumerated peripheral atoms, or, in other words, the peripheral bond connected to the peripheral atom in question which extends in the peripheral direction which is opposite to that of ascending enumeration.

EXAMPLE:

(2)



The atom concerned is atom "10". The peripheral bond which determines which of atoms "11" and "13" is first enumerated is the bond connecting atoms "9" and "10". The next succeeding peripheral ring after the 9-10-11-12 ring is the 13-14-15 ring, which accounts for the 13-14-15 enumeration. It is to be remembered that any ring which contains a peripheral atom is a peripheral ring. In all such cases the next succeeding peripheral ring after the ring containing the described peripheral bond is that ring which includes both of the fused faces to which the peripheral atom in question is common. See Sec. 5.5 for ciphering of the configurations involved.

5.23 Systems in Which All Peripheral Atoms are Fused

The order of ascending enumeration of the following ring systems:

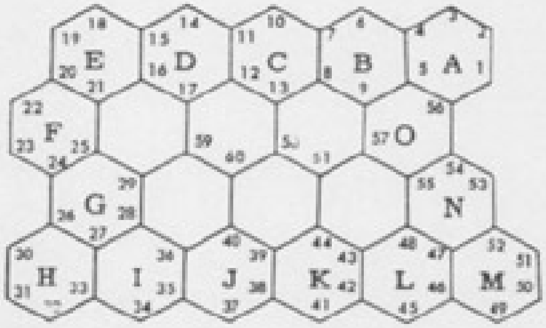
(1)

(2)

proceeds by successive peripheral rings in the same manner as described above. Unenumerated interior atoms are enumerated as occurring in that peripheral ring which contains (1) such atoms (2) the latest enumerated peripheral atom, and (3) the peripheral bond which extends from such peripheral atom in the direction opposite to that of ascending enumeration.

5.24 Systems Having Interior Atom(s) Not Part of a Peripheral Ring.

Whenever unenumerated ring atoms remain after all atoms of the peripheral rings have been enumerated, enumerate (and cipher) such remaining atoms in the ascending numerical order of the enumerated atoms to which such atoms are bonded, continuing at each instance the ascending numerical sequence with the next higher unused number.

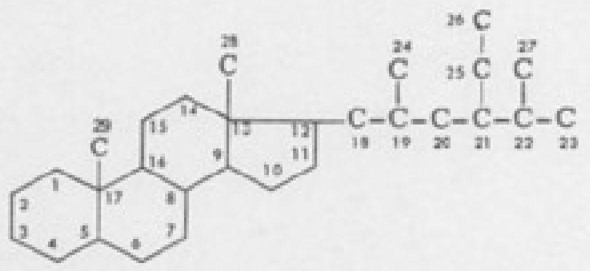


6L3YyLYyyLYyy,yLYyy,yLLYyLLYyYyyyL3
YLYyLYyy,yLYyy,yLYyyL3YLYyY--y

5.3 ASCENDING ORDER OF ENUMERATION OF SKELETAL SUBSTITUENTS

Skeletal substituents, necessarily acyclic, are enumerated as though branches of an open chain after the enumeration of all ring atoms, and in the ascending numerical order of the ring atoms to which such substituents are bonded, in the manner already set forth for monocyclic compounds in Sec. 4.1.

EXAMPLE:



6L4YLLYY5LLL(CCMCCET)YMLLYYM

5.4 SELECTION OF CORRECT STARTING ATOM AND PERIPHERAL DIRECTION OF ASCENDING ENUMERATION

Begin the enumeration with that ring atom and continue to enumerate in that constant peripheral direction (clockwise or counterclockwise) which generates the ascending order of enumeration, in accordance with the procedure described in Sec. 5.20-5.30, which assigns the lower number on the occasion of the first difference to the following features listed in their order of decreasing priority:

1. ring atom to which is bonded the
   - a. greater number of hydrogen atoms in the saturated hydrocarbon substituent free state of the ring system;
   - b. greater number of skeletal substituents;
   - c. skeletal substituent having the
     - (1) greater number of skeletal atoms;
     - (2) ascending enumeration pattern of the saturated hydrocarbon state which assigns the lower number on the occasion of the first difference to carbon atom which bears the greater number of hydrogen atoms;
2. features described by the updating rule (Sec. 2.61) in their same order of priority.

The requirement of feature 1a., above, compels the enumeration to start with an unfused (peripheral) atom, whenever one exists, since all unfused atoms of a saturated hydrocarbon unsubstituted fused ring system bear two hydrogen atoms, which is at least one more hydrogen atom than is borne by any fused atom.

At the outset any unfused ring atom is a potential starting atom, and each such atom remains in contention for selection as starting atom until eliminated by another contender, according to the described selection rule. Fortunately, the field can be narrowed down quickly to a very few contenders since the correct starting atom in order to qualify on the basis of feature 1a. must always, where there is a difference,

(1) occupy the ring having the greater number of unfused atoms, and

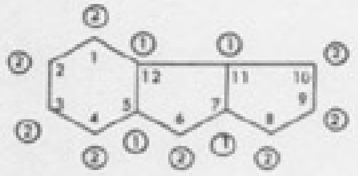
(2) occupy a ring position which is one bond removed from a fused atom.

In the following discussion the expression "path first richer in hydrogen" is intended to be merely a more succinct statement of the expression "sequentially enumerated path of carbon atoms whose ascending enumeration pattern assigns the lower number on the occasion of the first difference to that carbon atom which bears the greater number of hydrogen atoms, as compared to a correspondingly enumerated carbon path".

EXAMPLES (saturated hydrocarbon ring systems):

In the following examples the number of hydrogen atoms (implied) bonded to each ring atom is indicated by an encircled number:

(1)



Beginning with the number 1 atom the correct enumeration shown generates 4 successive ring atoms, each having two hydrogen atoms attached. The only other path equally rich in hydrogen at each successive ring position is the 4-3-2-1 path. Addition of another atom, in the generating direction, to each path gives each path five atoms defined as follows:

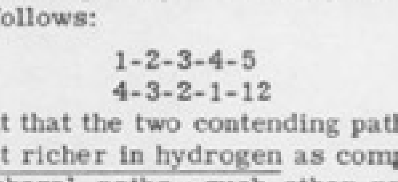
1-2-3-4-5
4-3-2-1-12

It is evident that the two contending paths are still equally first richer in hydrogen as compared to all other peripheral paths, such other paths having been eliminated from contention after the first four generated positions, as indicated above. Addition of one more atom to each generating path defines the two paths as follows:

1-2-3-4-5-6
4-3-2-1-12-11

At this point the 1-6 path becomes richer in hydrogen at atom 6 than the contending 4-3-2-1-12-11 path thus to become that sequentially enumerated path of the ring system which becomes first richer in hydrogen.

(2)



Upon inspection of the steroid nucleus above it becomes evident that the 1-2-3-4 and 4-3-2-1 paths become equally richer in hydrogen at lower numbered path positions than any other four atom ring path. Addition of two more carbon atoms to each of the contending paths in the respective generating directions gives the paths the following atom definitions:

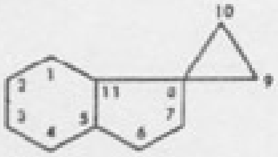
1-2-3-4-5-6
4-3-2-1-17-16

Positions 6 and 16 are decisive since position "6" enriches its path by 2 hydrogen, whereas the correspondingly generated position 16 enriches its path by only one hydrogen. The number "1" ring atom therefore generates, in the direction shown by the enumeration, that serially enumerated path which becomes first richer in hydrogen.

NOTE: The term "generates", as used in this notation, means "establishes according to the prescribed order of enumeration".

SPIRO RING CONTAINING:

(3)



6L4Y5LLX3LL-Y

NOTE. Spiro rings are not free to rotate and are enumerated in the same constant peripheral direction as ortho-fused atoms, as already explained.

Where two or more potential starting atoms of a saturated hydrocarbon system generate paths which are equally first richer in hydrogen, with respect to all other generated ring paths, at each successive ring atom generated, such paths are symmetrical and any one of such starting atoms may begin the enumeration without ambiguity.

In the following formulas those starting atoms which generate paths equally first richer in hydrogen at all corresponding (equal number of enumerated atoms from starting atom) path positions are labelled by asterisks. The arrows show the related directions of generation:

NON-CONDENSED SYSTEMS:

(4)

6L4Y5L3Y

Ciphering of the atoms of either formula in numerical order gives the same unique cipher.

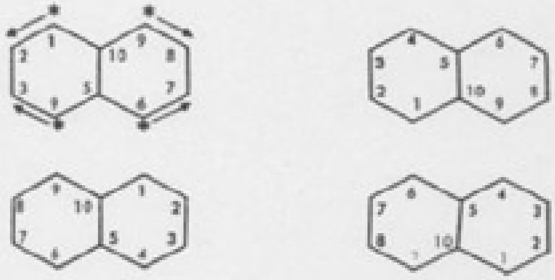
(5)

Either asterisked atom may begin the enumeration in the direction shown to produce the unique cipher:

6L4YLLYL4YY

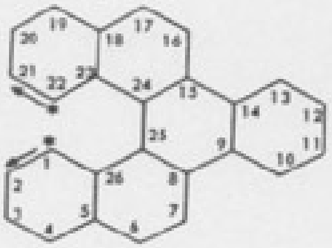
Other geometrically identical enumerations are shown below:

(6)



All of the naphthalene (saturated) enumerations shown above are equivalent and produce the same cipher: 6L4YL4Y

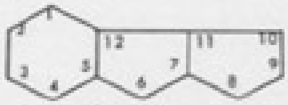
(7)

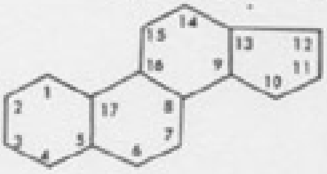


6L4YLLYYL4YYLLYL4YYYY

5.41 Derivatives

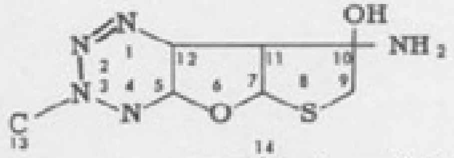
If the configuration of the parent system is such that there exists only one permissible atom starting as, in the following cases:



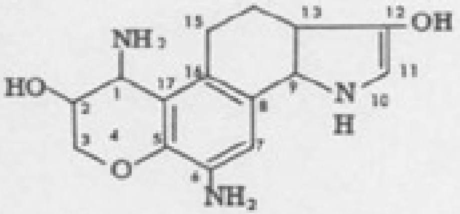


the enumeration pattern is inherently unique and serves directly for all of its derivatives without regard to the nature or distribution of derived features, as long as no other ring system is added which would itself control the enumeration as described in the section relating to ring assemblies. Derivatives of the foregoing parent systems are enumerated below:

(1)



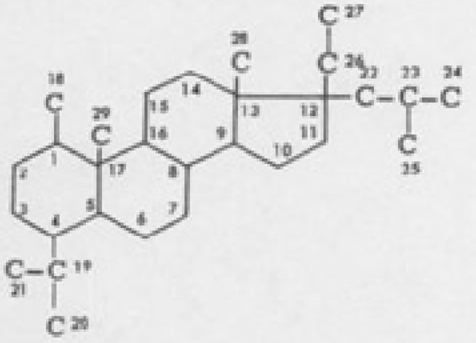
(2)



In the following examples the stated feature is that which reduces the number of contending starting atoms to one.

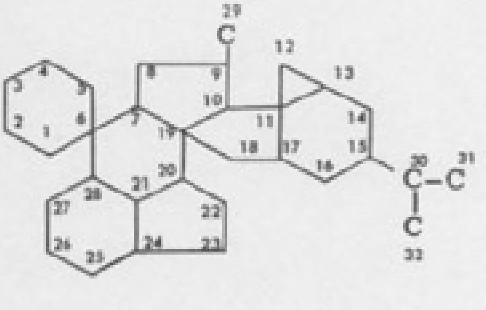
EXAMPLES (feature 1a of Sec. 5.4 decisive):

(3)



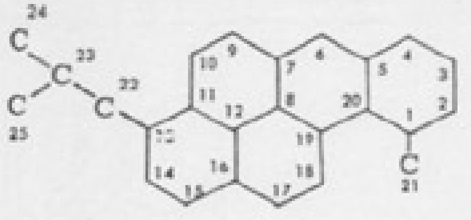
6LMLLLTYLLYY5LLL(CT)EYMLLYYM

(4)



$\text{6L5}\overset{6}{\text{X}}\text{Y5LLMY5}\overset{11}{\text{Y}}\text{6,3LYLLLTLY5L}\overset{19}{\text{Y}}\text{5,6Y}\overset{21}{\text{5}}\text{yLLYL3}\overset{28}{\text{Y}}$

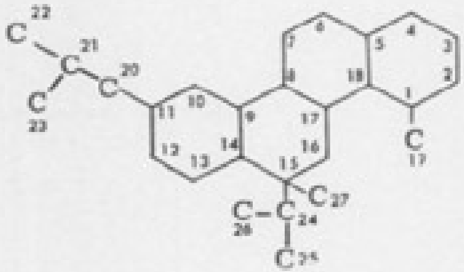
(5)



$\text{6LML3YLY}\overset{8}{\text{Y}}\text{yLLY}\overset{12}{\text{y}}\text{L(CT)LL}\overset{16}{\text{Y}}\text{LLYY}$

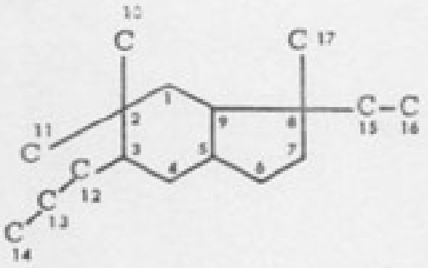
EXAMPLES (feature 1b. of Sec. 5.4 decisive):

(6)



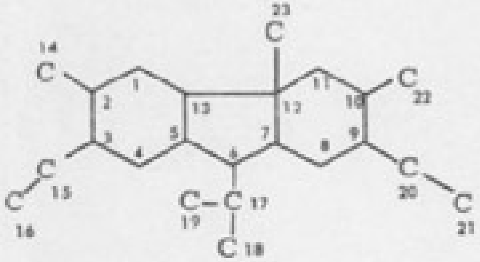
6LML3YLLYYLL(CT)LLYLTMLYY

(7)



6LLM2L(C3)LY5LLLEMY

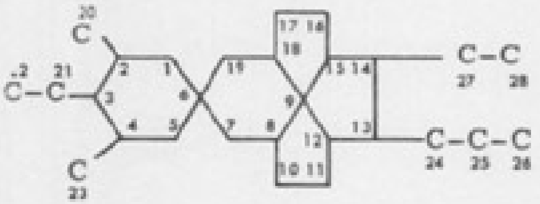
(8)



6LLMLELY5LTYLLELMLY5MY

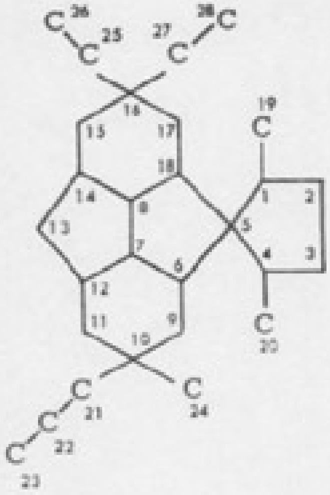
EXAMPLES (feature 1c(1) of Sec. 5.4 decisive):

(9)



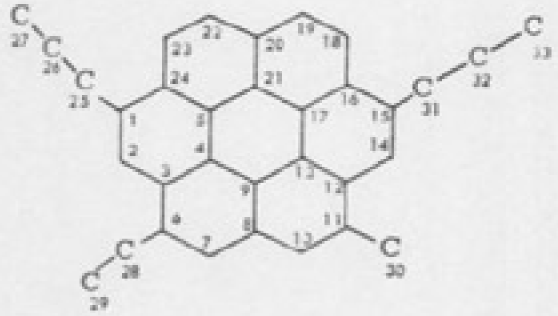
6LLMLELMLXLY5y5,5LLY5L(C3)LEY5LLYL

(10)



5LMLLLM$\overset{5}{\text{X}}$5Yy5yLL(C3)ML$\overset{12}{\text{Y}}$5L$\overset{14}{\text{Y}}$LLE2LY5

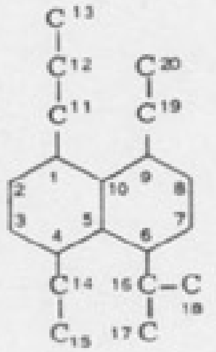
(11)



6L(C3)LYyyLELYyLLMYyLL(C3)YyLLY$\overset{21}{\text{y}}$LLY

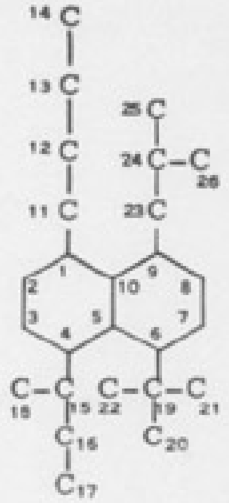
EXAMPLES (feature 1c(2) of Sec. 5.4 decisive):

(12)



6L(C3)LLLEYLTLLLEY

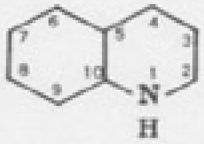
(13)



6L(C4)LLL(CME)YL(CM3)LLL(CT)Y

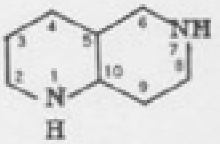
EXAMPLES (feature 1 of Sec. 2.61 decisive):

(14)



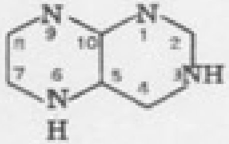
6nHLLLYL4Y

(15)



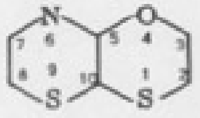
6nHLLLYLnHLLY

(16)



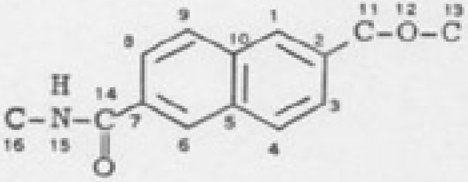
6nHLnHLYnHLLnHY

(17)



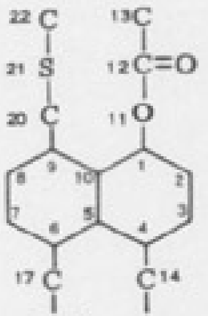
6SLLOYnHLLSY

(18)



6RR(COM)RRYRR(CVNHM)RRY

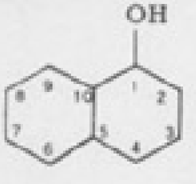
(19)



6L(OCVM)LLL(COM)YL(CNHM)LLL(CSM)Y

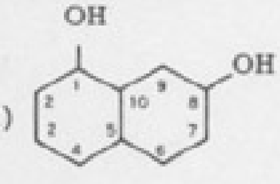
EXAMPLES (feature 2a.of Sec. 2.61 decisive):

(20)



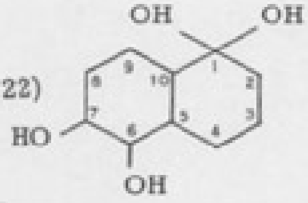
6LQL3YL4Y

(21)



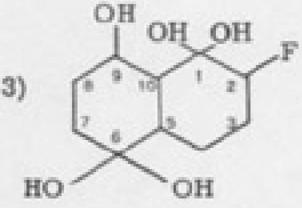
6LQL3YLLLQLY

(22)



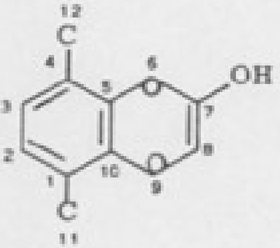
6LQ2L3YLQLQLLY

(23)



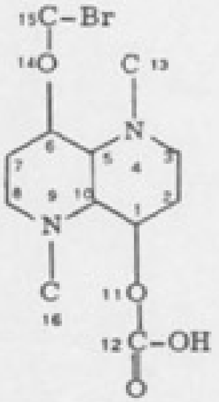
6LQ21.FLLYLQ2LLLQY

(24)



6RMRRRMYOLQ:LOY

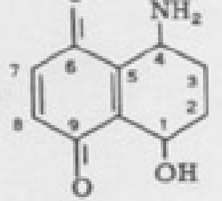
(25)



6L(OCVQ)LLnMYL(OCB)LLnMY

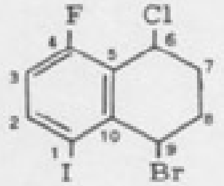
EXAMPLES (feature 2b.of Sec. 2.61 decisive):

(26)



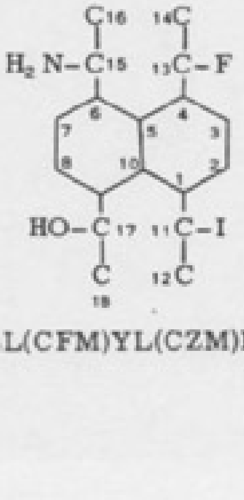
6LQLLLZY {:} LVL:LLVY

(27)



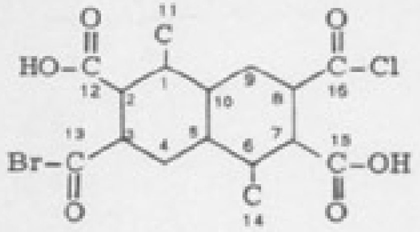
6RIRRRFYLKLLLBY

(28)



6L(CIM)LLL(CFM)YL(CZM)LLL(CQM)Y

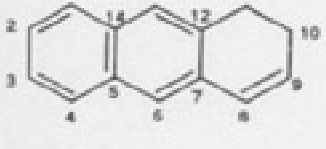
(29)



6LML(CVQ)L(CVB)LYLML(CVQ)L(CVK)LY

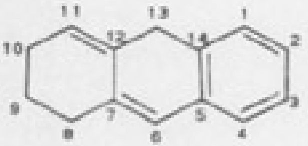
EXAMPLES (feature 2c.of Sec. 2.61 decisive):

(30)



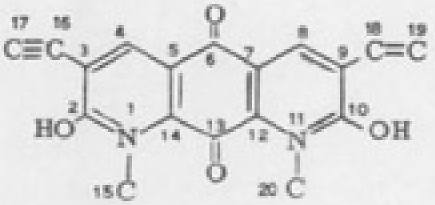
6R4YRYL:LLLYRY

(31)



6R4YL:YL3L:YLY

(32)



6nMRQR(C+C)RYLVYRR(C=C)RQnMYLVY

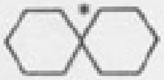
If, after all of the above criteria have been exhaustively applied, a plurality of potential starting atoms and/or directions remain in contention, begin the enumeration with any one of such remaining contenders.

5.5 CIPHERING. SYMBOLS. R,L,X,Y

Unfused carbon atoms of L-type rings are ciphered by "L"; unfused atoms of R-type rings, by "R" in the manner already described for monocyclic ring carbon atoms.

Carbon atoms which occupy peripheral fused ring positions, other than spiro-fused, are ciphered by the capital letter "Y". The two arms, which point in the peripheral direction of ascending enumeration, and the leg of the Y, which extends in the opposite direction, symbolize the three paths (bonded directions) which diverge from a fused atom as in naphthalene:

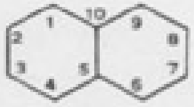
The capital letter "X" represents a spiro carbon and symbolizes the four ring paths which branch from a spiro atom:



When a Y atom is ciphered, suffix the Y by a number equal to the size of the ring embraced by the arms of the Y, if the ring is other than 6 membered. The bond connecting the Y atom with the next lower numbered ring atom forms the leg of the Y. If no number follows a Y symbol the arms are understood to embrace or introduce a 6 membered ring.

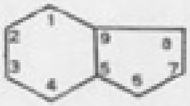
EXAMPLES:

(1)



6L4YL4Y

(2)

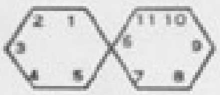


6L4Y5L3Y

Suffix each X symbol by a number equal to the size of the ring embraced by the angle of the X in the direction of the next higher numbered ring position, if the size of the ring so embraced is other than 6 membered. Absence of a numerical suffix after an X implies a 6 membered ring is introduced.

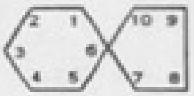
EXAMPLES:

(3)



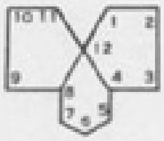
6L5XL5

(4)



6L5X5L4

(6)

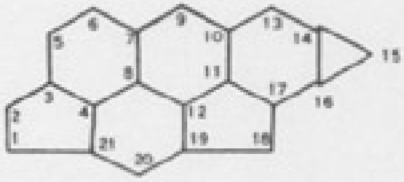


5L3YL3Y5L3Y6,5 (See 5.52)

5.51 Interior Fused Atoms. Symbol "y"

The small letter "y" is used to denote an interior fused atom with the same "arm" and "leg" significance as described for the capital Y. The size of the ring embraced by the arms of the y atom immediately suffixes the "y" if the ring is other than 6 membered. Absence of a number after a "y" symbol implies that the ring introduced by the y atom is 6-membered.

EXAMPLE:



5LLYyLLY$\overset{8}{y}$LY$\overset{11}{y}$5$\overset{12}{y}$L$\overset{14}{Y}$3L$\overset{16}{Y}\overset{17}{Y}$5L$\overset{18}{Y}$LY5

5.52 Quaternary Ortho Fused Atoms

When four bonds radiate from a Y or y atom so that two pairs of arms extend from the same leg suffix the Y or y symbol by the sizes (in all cases) of the two rings which are embraced by the two pairs of arms citing first the size of the ring which is ortho fused to the ring which contains the leg. Separate the ring sizes by a comma. Sec. 5.22(1).

5.53 Multiplication of Ring Atoms

A continuously bonded series of three or more "R" atoms or "L" atoms which are

(1) not substituted and

(2) not bonded to a ring hetero atom (or multiple bond, if L atom) are ciphered, respectively, by a single R or L suffixed by the number of such atoms in the series. The R atoms so multiplied represent $\overset{H}{-C=}$ configurations only; the L atoms, $-CH_2-$ only.

5.54 Hetero Atoms Occupying Fused Positions

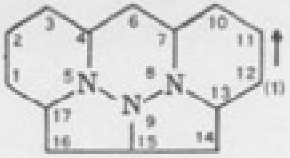
When a hetero atom occupies a fused position which would be ciphered by X,Y, or y if the position were occupied by a carbon atom, the hetero atom is ciphered by its normal symbol (see Symbol Tables) and suffixed by the appropriate carbon atom symbol, (X,Y, or y) including ring size—if other than 6, enclosed by parentheses.

EXAMPLES:

(1)

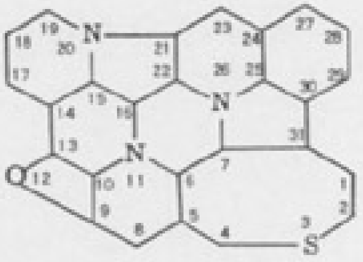
6L4n(Y5)LYL4Y5Y

(2)



6L3Yn(y5)LYn(y5)n(y5)L3Y5LY5LY

(3)



8LLSLYyy5LY4yn(y)OYYy5yL3n(Y5)YyLYy5n(y)L3
Y5Y8

5.55 Symbols. Multiple Bonds. Ciphering.

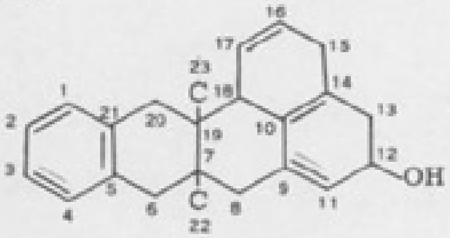
A double bond between atoms of a fused face which does not comprise an R ring, is represented by a colon enclosed within braces {:} , placed after the cipher of that one of its connected atoms which occurs on or nearer the periphery.

A double bond between atoms, at least one of which is not fused, of an "L" type ring is ciphered by a colon without parentheses ":".

A double bond represented by {:} , as described above, is ciphered after citation of the fused atom "Y" and ring size, if expressed.

EXAMPLES:

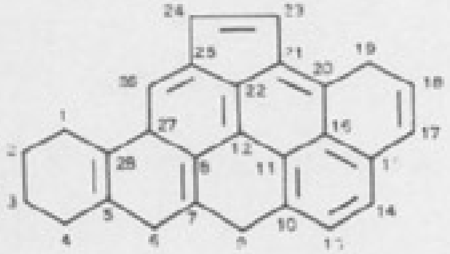
(1)



cipher: 6R4$\overset{\bullet}{Y}$LYMLYy:LLQLY {:} LL:$\overset{18}{Y}$YMLY

*NOTE that the 5-21 interface is part of an "R" ring so that the 5-21 double bond is not ciphered, whereas the 10-14 double bond is not part of an "R" ring and is ciphered as shown.

(2)



6L4$\overset{5}{Y}$ {:} L$\overset{7}{Y}$ {:} $\overset{8}{y}$L$\overset{10}{Y}\overset{11*}{y}r\overset{12}{y}$RRYyL:LL$\overset{20}{Y}\overset{21}{Y}5\overset{22}{y}$ {:} RRY:LYY

*See next paragraph

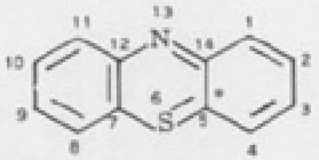
5.56 "R"—Rings Having No "R" Atoms

When all atoms of a ring are ortho-fused or the ring is so composed of hetero atoms that no unfused position is occupied by a carbon atom, cipher the (lowest numbered) atom of such ring by placing after the regular symbol of such atom the lower case letter "r" if the ring is an "R" ring. Absence of the "r" placed as described, denotes the ring as being of the "L" type.

In the following examples the lowest numbered atom of the type of ring in question is indicated by an asterisk.

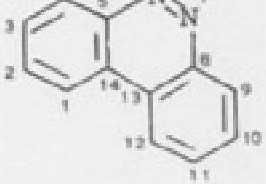
EXAMPLES:

(1)



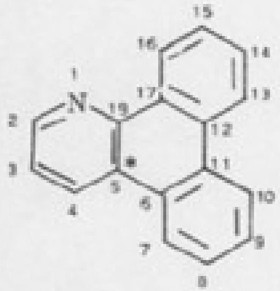
6R4YrSYR4YnY

(2)



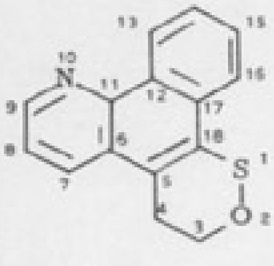
6R4YrnnYR4YY

(3)



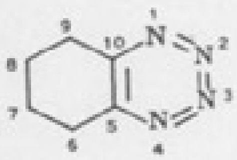
6nRRRYrYR4YYR4YY

(4)



6SOLLYrYRRRnYYR4YY

(5)



6nrnnnYL4Y

6.0 BRIDGED RING SYSTEMS. DEFINITION

A bridged ring system is characterized by the following features

(1) contains at least one ring interface of three or more atoms,

(2) does not contain two ring interfaces, as described by (1), which together comprise a ring larger than the aggregate sum of the atoms and bonds contained in the two interfaces.

Feature 2 merely establishes the condition that the molecule must not be classifiable as a circular ring assembly, as defined in Section 7.61.

The increased order of complexity over fused ring aggregates which is exhibited by bridged ring aggregates is due to the characteristic presence in the latter of two rings which have more than two atoms in common. By the stated structural feature the configuration of bridged ring systems transcends the bounds of plane geometry and moves into the third dimension thereby making it quite difficult to represent the molecule by a systematic planar diagram as discussed in Sec. 6.2.

6.1 NOTATION SYMBOLS. ASTERISK "*". NUMERALS IN PARENTHESES (1), (2), . . . DELTA "Δ"

The asterisk is used as a dummy symbol to introduce the cipher of each bridge.

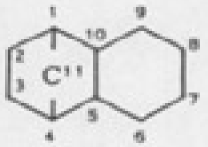
The symbol "Δ" is used as a dummy symbol to introduce a bridge branch.

An arabic numeral in parenthesis is used to symbolize the end of a bridge or bridge branch, the symbol "(1)" for the first occasion and the number increased by 1 for each successive occurrence. The same parenthesized numeral used to signal the end of a given bridge, or branch thereof, if used to suffix the symbol of the parent system atom to which the end concerned is connected.

The following examples illustrate the use of the newly introduced symbols.

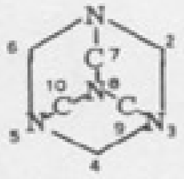
EXAMPLES:

(1)



$6\overset{1}{L}*\overset{11}{L}(1)LL\overset{4}{L}(1)YL4Y$

(2)



$6n*\overset{7}{L}\overset{8}{n}\Delta\overset{9}{L}(1)\overset{10}{L}(2)L\overset{3}{n}(1)Ln(2)L$

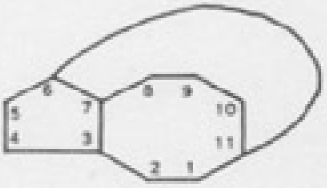
Note that each bridge is ciphered as though a substituent of the lowest numbered atom of the parent system to which the bridge is bonded. In formula (2) atoms 7-10 constitute a single bridge, which is branched.

6.2 ESTABLISHMENT OF THE PLANAR DIAGRAMS OF BRIDGED RING SYSTEMS

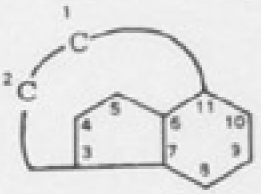
The planar diagrams of cyclic compounds whose ring systems consist solely of single rings and/or fused ring aggregates offer little graphic confusion and are represented in this notation in conventional fashion (hydrogen attached to carbon being implied).

The planar representation of compounds which contain ring interfaces of three or more atoms, three dimensional structures, and/or crossed bonds is not so straightforward and has been largely subjective and arbitrary. In many such planar representations it is difficult to determine the number of rings contained in a given structure, or to distinguish between a ring and a bridge thereof, and in a number of cases even to recognize two different representations as the same compound, as illustrated by the multiple representations of the three compounds below, the arabic numerals showing correspondence between atoms of the equivalent structures indicated by alphabetic series:

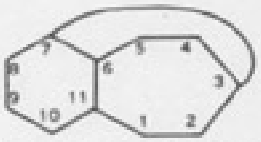
(1) A.
RRI 2688



B.

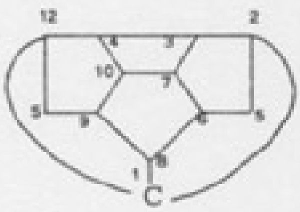


C.

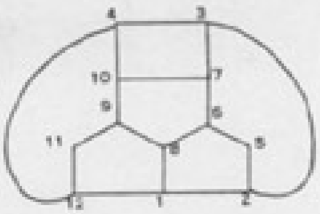


7LLL*(1)LLYL(1)L3Y7

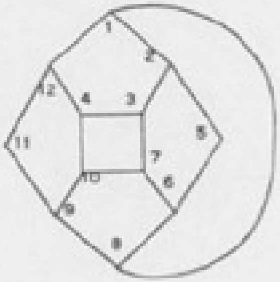
(2) A.
RRI 6550



B.

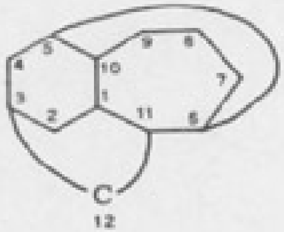


C.

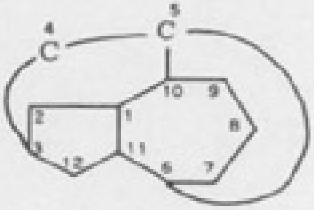


5L*(1)Y5y4y5LY5y4L(1)Y5y4LY5

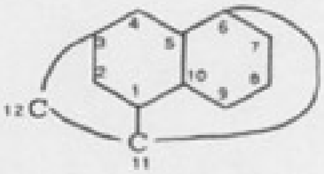
(3) A.



B.



C.



6L*LδL(1)(2)LL(1)LYL(2)L3Y

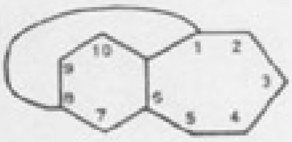
Structures (1)c., (2)c., and (3)c. are the systematic planar diagrams of this notation, as explained below.

In an attempt to overcome the stated difficulties a procedure is described which serves to establish an unambiguous and systematic planar configuration for every ring system in either the saturated hydrocarbon or any derived state. According to this procedure each bridged ring system is expressed as a derivative of a parent single ring or ortho and/or spiro fused ring system. The parent ring system is considered to occupy the reference plane (plane of paper) while any remaining ring paths-atoms and/or bonds-are characterized as bridges which lie outside of the reference plane.

When an unsubstituted bridged system contains no quaternary or directly connected ternary atoms, i.e. contains no potentially planar ortho or spiro fused faces, the planar parent ring system is a single ring. When the bridged system contains one or more ortho or spiro fused faces, the parent system is a fused ring aggregate.

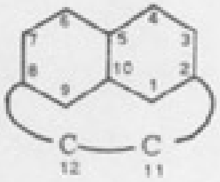
EXAMPLES (Parent systems indicated by geometric polygons):

(4)



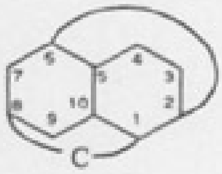
7L*(1)L4YLL(1)LLY7

(5)



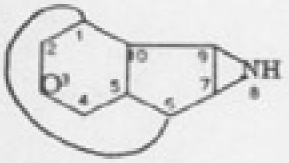
6LL*LL(1)LLYLLL(1)LY

(6)



6L*L(1)L*(2)LLYL(2)LL(1)LY

(7)



6L*(1)LOLY5L(1)Y3nHY5Y

6.3 ESTABLISHMENT OF THE PLANAR PARENT RING SYSTEM

It is normally possible, by bending stretching and twisting bonds, to establish from a given bridged ring system a number of planar ring systems which are eligible contenders for selection as parent system. In the formation of the various possible planar systems for consideration as parent it is permissible to stretch, bend, or twist bonds in any direction so long as such bonds are not broken. However, after an eligible ring system has been established in the reference plane for consideration as parent system, all of its atoms and bonds are considered as fixed to the plane and not shared by any other ring except by ortho and/or spiro fusion in the same plane. Any ring configuration, atom or bond, which can be deleted from the structural formula without rupturing a ring of an established planar system is a bridge or part of a bridge of such contending system.

It is essential to keep in mind that the parent planar ring system, by declaration as a law of the system, must be a single ring or a fused ring aggregate. Consequently, no ring interface of three or more atoms is allowed to exist (logically) in the reference plane.

When the parent ring system is a fused ring aggregate, a bridge may be constituted by any configuration of atoms and bonds and may consist of a bond only.

6.4 SELECTION OF THE CORRECT PARENT RING SYSTEM

Select as the parent ring system of a given bridged ring compound that eligible (single ring or fused ring aggregate) planar ring system which exhibits the following features listed in their order of decreasing priority:

1. greater number of
    - a. fused rings
    - b. ortho fused faces
    - c. six-membered rings
    - d. ring atoms
2. ascending enumeration pattern which assigns the lower number on the occasion of the first difference to the features listed in Sec. 6.7 and in their same order of priority.

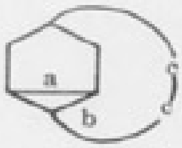
In the event of a tie on the basis of all of the listed features the contending parent systems which establish the tie are symmetrically disposed with respect to such features so that any one of such systems may be selected as the parent system without ambiguity.

EXAMPLES. In the following examples the various different fused ring aggregates which can be established from a given bridged ring system are shown in alphabetical series of capital letters. All bonds between ternary and/or quaternary atoms, which represent potential fused faces, are labelled by identifying small letters to show correspondence among the different structures of a given series. Fused ring aggregates are shown as geometric polygons; the bridges, as individually expressed atoms and/or bonds. The final decisive feature - of Sec. 6.4 - for its selection is shown opposite each correct parent ring aggregate. "RRI" indicates Revised Ring Index number.

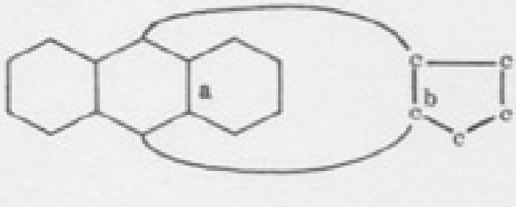
(1) A.
RRI 2095

1.c.

B.

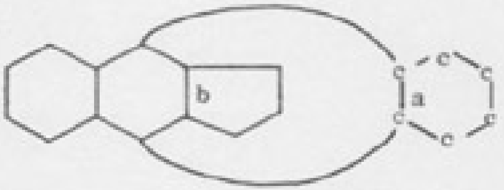


(2) A.
RRI 5854

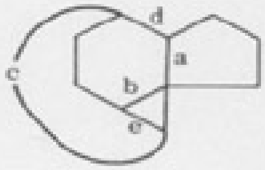


1.c.

B.

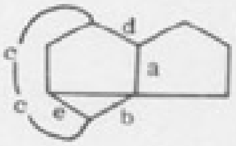


(3) A.
RRI 3967

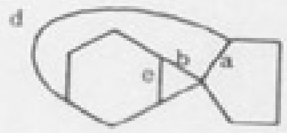


1.c.

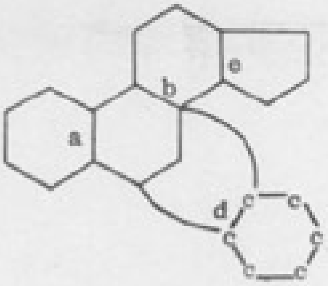
(3) B.



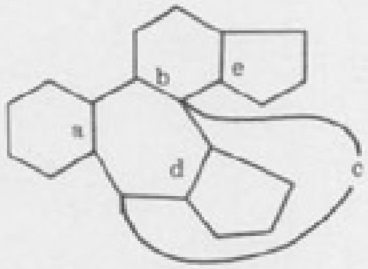
C.



(4) A.
RRI 6597

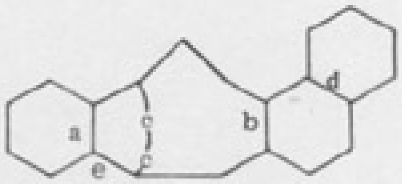


B.



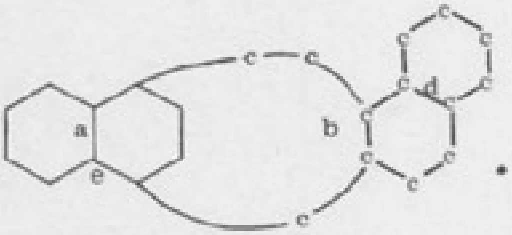
1.a.

(5) A.
RRI 6456

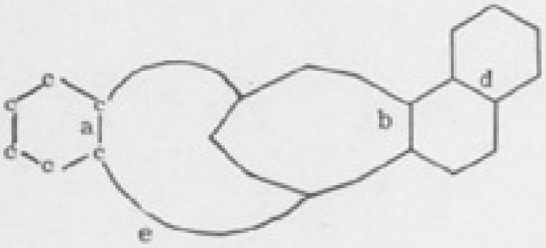


1.a.

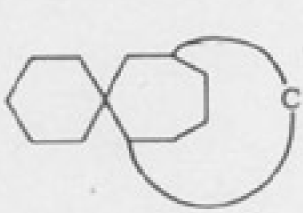
B.



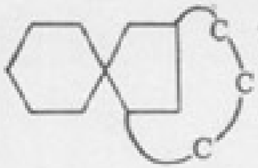
C.



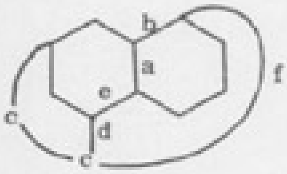
(6) A.
RRI 2776



B.

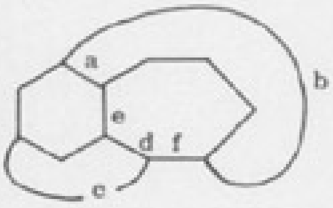


(7) A.

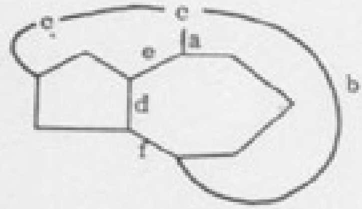


1.c.

B.

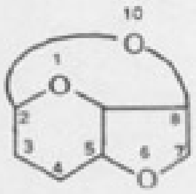


C.



In the following examples the contending forms have been omitted: The correct systematic formula is shown.

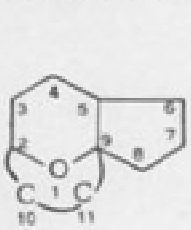
(8)
RRI 2418



1.c.

6OL*O(1)LLY5OLL(1)Y

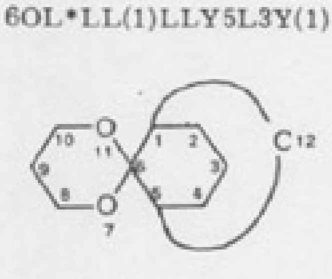
(9)
RRI 2501



1.c.

6OL*LL(1)LLY5L3Y(1)

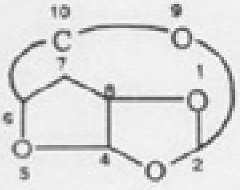
(10)
RRI 2543



1.c.

6L*L(1)LLL(1)LXOLLLO

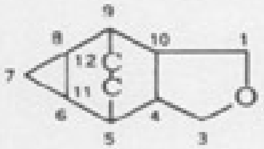
(11)
RRI 2566



1.a.

5OL*OL(1)OY5OL(1)LY5

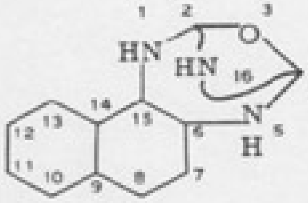
(12)
RRI 3984



1.a.

5LOLYL*LL(1)Y3LYL(1)Y5

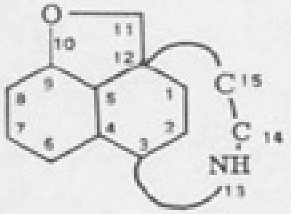
(13)
RRI 4034



3.

7nHL*nH(1)OL(1)nHYLLYL4YY7

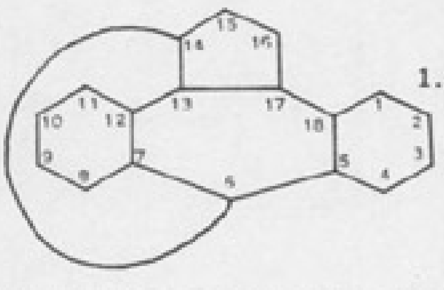
(14)
RRI 4615



1.c.

6LLL*nHLL(1)Yy5L3Y5OLY(1)

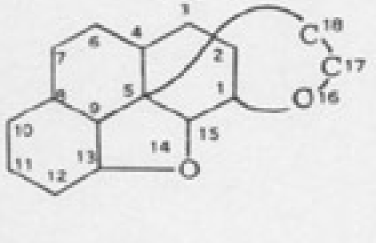
(15)
RRI 5701



1.a.

6L4Y7L*(1)YL4Y7Y5L(1)LLY7Y

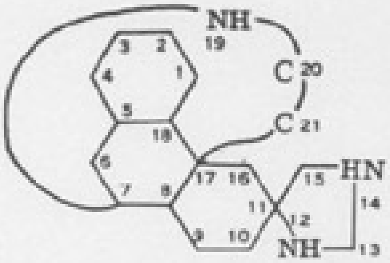
(16)
RRI 5822



1.a.

6L4YLL*nHLL(1)YLLX5nHLnHL-LY(1)Y

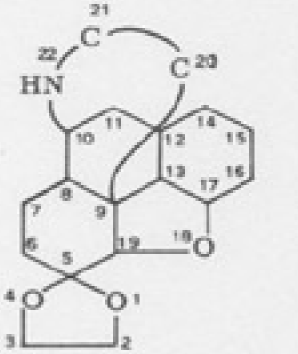
(17)
RRI 5931



1.b.

6L*OLL(1)LLYy5(1)LLYy5L3Y5OY

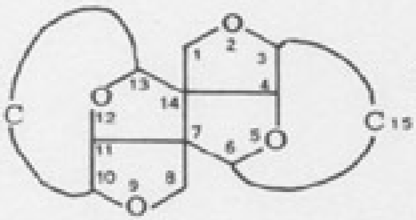
(18)
RRI 6620



1.b.

5OLLO$\overset{5}{\text{X}}$LLY$\overset{9}{\text{y}}$5*LLnH(1)$\overset{10}{\text{L}}$(1)LY$\overset{13}{\text{y}}$5L3Y5OY

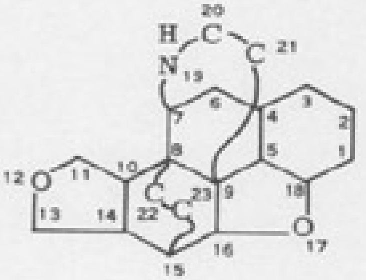
(19)
RRI 6557



1.b.

5LOL*L(1)Y5OL(1)Y5,5LOL*L(2)Y5OL(2)Y5,5

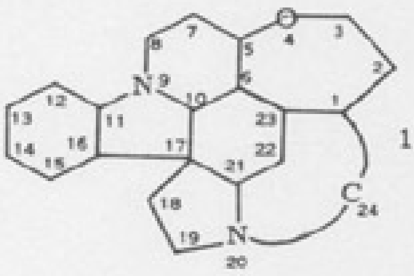
(20)
RRI 7144



1.b.

6L3Y$\overset{5}{\text{y}}$5LL*$\overset{14}{\text{n}}$HLL(1)$\overset{8}{\text{Y}}$*LL(2)$\overset{4}{\text{y}}$5(1)Y5LOLYL(2)
Y5OY

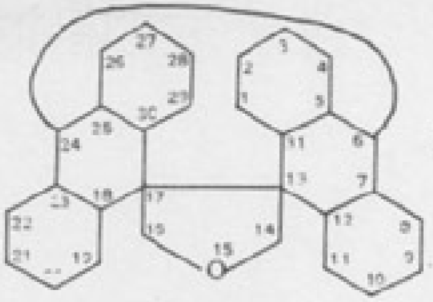
(21)
RRI 7172



1.a.

7L*L(1)LLOYyLLn(Y5)yYL4Y5Y6,5LLn(1)YLY7

(22)
RRI 7474

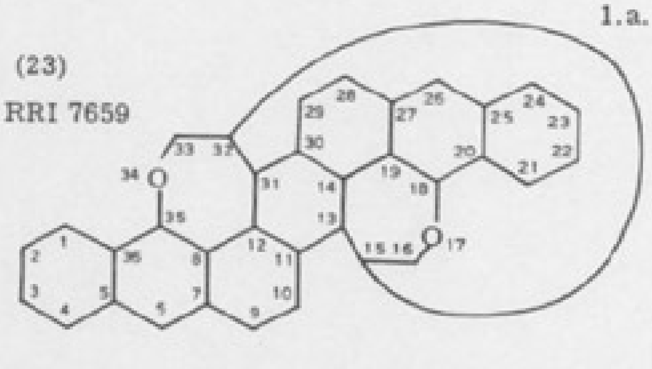


1.a.

6L4YL(1)YL4YX5LOLXYL4YL(1)YL4Y--Y

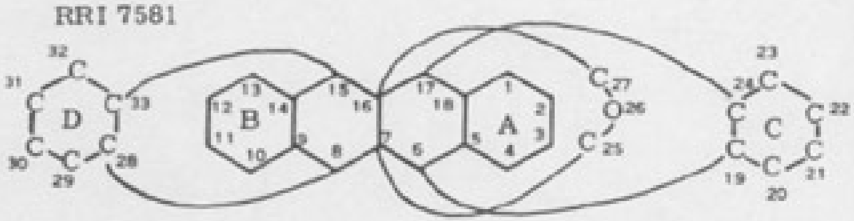
(23)
RRI 7659

1.a.



6L4YLYy7LLYy7Y7yL(1)LOYyYL4YLYLLYY
7L(1)LOYY

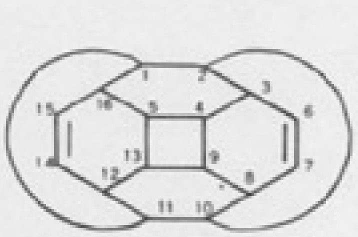
(24)
RRI 7581



6L4YL*YL4Y(1)Y*LOL(2)L*YL4Y(3)YL4YL(3)
Y(2)L(1)Y

In the above system, because of symmetry, ring "C" is interchangeable with ring "A"; and ring "D", with ring "B" for inclusion in the reference plane.

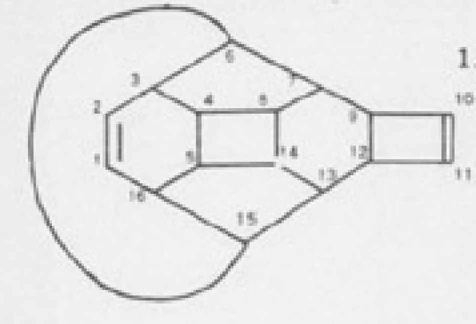
(25)
IUPAC, 1958
pp. 146-8



1.a.

6L*(1)L*(2)Y$\overset{4}{\text{y}}$4$\overset{5}{\text{y}}$L:LY$\overset{9}{\text{y}}$4L(2)L(1)Y$\overset{13}{\text{y}}$4L:LY

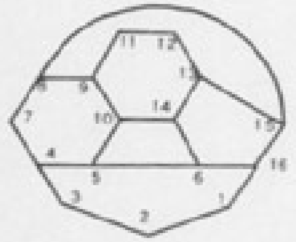
(26)



1.a.

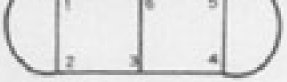
6L:LY5$\overset{4}{\text{y}}$4$\overset{5}{\text{y}}$5L(1)Y$\overset{8}{\text{y}}$4Y4L:LYY5$\overset{14}{\text{y}}$4L(1)Y

(27)



7L3Y$\overset{5}{\text{y}}$4$\overset{6}{\text{y}}$5LL*(1)Y$\overset{10}{\text{y}}$4LLY5$\overset{14}{\text{y}}$4L(1)Y7y4

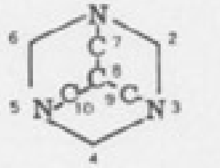
(28)



L*(1)L*(2)Y4L(1)L(2)Y4

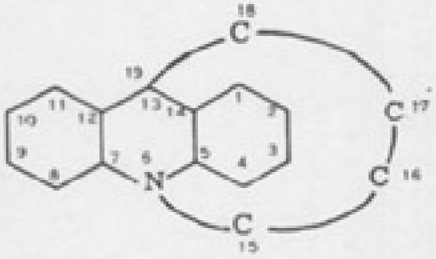
In the selection of the planar parent system of a bridged ring system which contains no potential ortho and/or spiro fused faces it is to be noted that only features 1c. and below of section 6.4 apply.

EXAMPLES:

	Ring Index entry	Systematic form
(1) RRI 3239		

The assignment of a higher priority to the greater number of six-membered rings-fused or single (one greater than none) - than to the greater total number of ring atoms allows "ansa" compounds (see Fieser and Fieser (loc. cit.), p. 322.) to be properly portrayed as a bridge derivative of the para positions of a six-membered ring, as illustrated by formula (2) below:

(2)
RRI 5319



6.5 ORDER OF ASCENDING ENUMERATION OF BRIDGED RING SYSTEMS

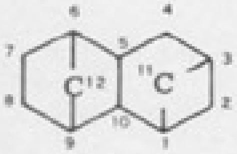
The configurations of a bridged ring system are enumerated in the following order of decreasing priority:

1. parent ring system;
2. bridges, in the manner described in Sec. 6.6.
3. skeletal substituents of the ring system, in the ascending numerical order of the bridged system atoms to which such substituents are bonded and in the event of a plurality attached to the same ring (or bridge) atom in the order set forth for substituents of an open chain; enumeration of each substituent proceeds from the ring outward and in the manner prescribed for open chains.

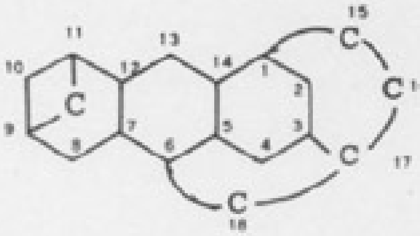
6.6 ENUMERATION OF BRIDGES

1. Enumerate bridges in the ascending numerical order of the lowest-numbered parent system atoms to which such bridges are bonded; and enumerate all atoms of a given bridge before proceeding to the next bridge in order.

EXAMPLES:



The "1" attached bridge is enumerated before the "6" attached bridge



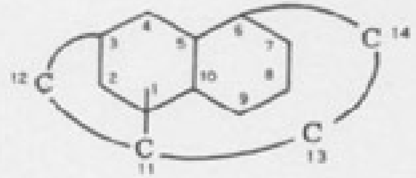
All four atoms of the bridge attached to "1" are enumerated before enumeration of the "9" bridge

2. Begin the enumeration of a bridge with that bridge atom which is directly bonded to the related lowest-numbered bridgehead atom and continue to enumerate the bridge atoms sequentially in the direction of the related highest-numbered bridgehead atom.

3. Begin the enumeration of each bridge with the next higher unused number remaining after enumeration of the parent system and of any earlier enumerated bridge.

4a. When a bridge is branched whereby it exhibits terminal bonds attached to more than two atoms of the parent aggregate, begin the enumeration as prescribed by rules 2 and 3 above. When a bridge atom is enumerated from which a plurality of unenumerated paths of bridge atoms branch, enumerate such branching paths in the ascending numerical order of the bridgehead atoms which terminate such branching paths.

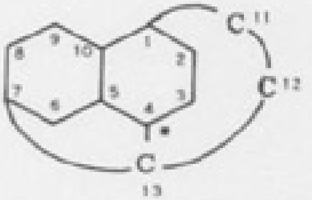
EXAMPLE:



6L*LΔL(1)LL(2)LL(1)LYL(2)L3Y

4b. When a branch of a bridge consists of a bond only, as indicated by the asterisk below, such branch does not affect the enumeration of the bridge.

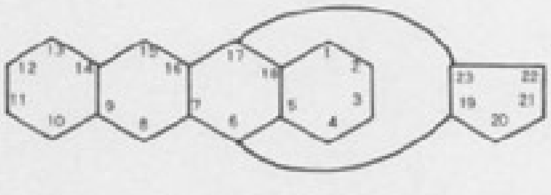
EXAMPLE:



6L*LLLΔ(1)(2)LLL(1)YLL(2)LLY

5. When a bridge is constituted by a ring system, enumerate around such system in that peripheral direction which proceeds from the lower numbered bridgehead atom toward the higher numbered bridgehead atom of the parent system. It is to be noted that the above definition of bridged ring aggregate requires that a ring system which is a bridge of a parent system must be joined to the parent system either by ortho or spiro fusion, although in a different plane from the reference plane. The same cipher symbols are used in the plane of the bridge as are used in the reference plane.

EXAMPLE:

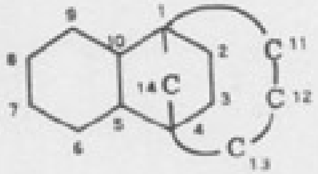


6L4YL•Y5L3Y(1)YLYL4YLYL(1)Y

6. When a plurality of bridges are bonded to the same lower numbered bridgehead atom, enumerate such bridges in the order in which they exhibit the following features listed in their order of decreasing priority:

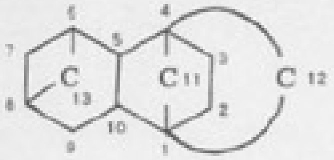
1. terminating bridgehead atom of lower number;
2. greater number of bridge atoms;
3. ascending enumeration pattern which assigns the lower number on the occasion of the first difference to the
   - a. bridge atom to which is bonded the
     - (1) greater number of hydrogen atoms in the saturated hydrocarbon unsubstituted state of the bridges concerned;
     - (2) greater number of skeletal substituents;
     - (3) skeletal substituent having the features described by items 2b(1) and (2) of Sec. 6.7;
   - b. heavier skeletal atom;
   - c. skeletal atom to which is bonded the features described by item 4 of Sec. 6.7.

(1)



6L•L3(1)•L(1)LLL(1)YL4Y

(2)



6L•L(1)•L(1)LLL(1)YLL•L(2)LL(2)Y

6.7 CORRECT STARTING ATOM AND PERIPHERAL DIRECTION FOR ENUMERATION

Begin the enumeration with that atom of the established parent ring system and continue to enumerate in that peripheral direction which generates the ascending enumeration pattern which assigns the lower number on the occasion of the first difference to the following features listed in their order of decreasing priority:

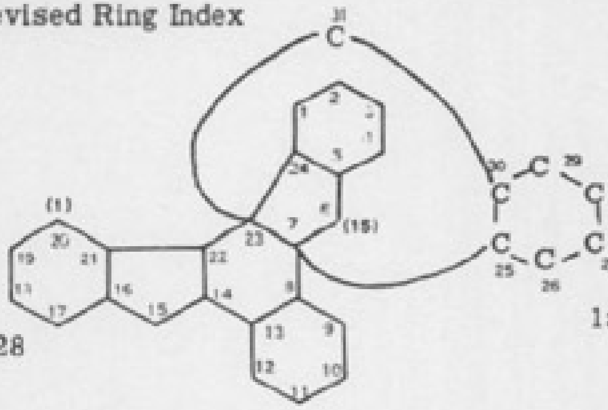
1. atom of the parent ring system to which is bonded the
   - a. greater number of hydrogen atoms in the saturated hydrocarbon bridge and substituent free state of the parent ring system;
   - b. greater number of bridges;
   - c. bridge having the
     - (1) greater number of bridge atoms;
     - (2) ascending enumeration pattern which assigns the lower number on the occasion of the first difference to the bridge atom which bears the greater number of hydrogen atoms in the saturated hydrocarbon unsubstituted state of the bridge;
2. ring or bridge atom to which is bonded the
   - a. greater number of skeletal substituents;
   - b. skeletal substituent having the
     - (1) greater number of skeletal atoms;
     - (2) ascending enumeration pattern of the saturated hydrocarbon state which assigns the lower number on the occasion of the first difference to the carbon atom which bears the greater number of hydrogen atoms;
3. features described by the updating rule (Sec. 2.61) in their same order of priority.

In bridged systems having a single ring as the parent ring system only features 1b. and below apply because of the complete symmetry of the parent ring.

In the examples below the ultimate decisive feature of Sec. 6.70 for selecting the starting atom is shown to the right of the formula concerned.

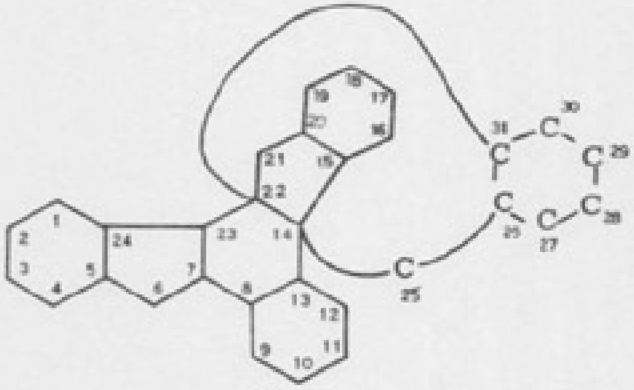
EXAMPLE: The formula A configuration (atoms 1-24) is the parent ring aggregate.

RRI=Revised Ring Index



(1)A.
RRI 7428

1a.

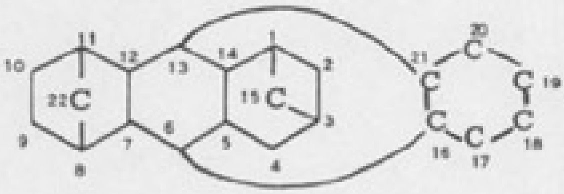


B

In formula A either atom "1" or atom "(1)" may begin the enumeration of the substituent free parent aggregate which becomes decisive at atom 15, or (15), when compared to formula B whose 15th atom bears one less hydrogen atom. Formula A is selected as the parent ring aggregate in accordance with Sec. 6.4 which incorporates the features of Sec. 6.7.

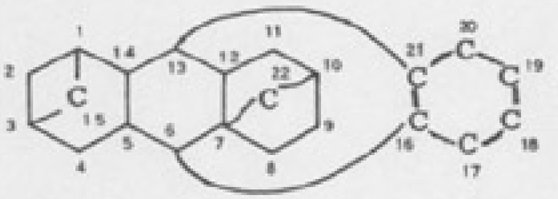
EXAMPLES:

(2)



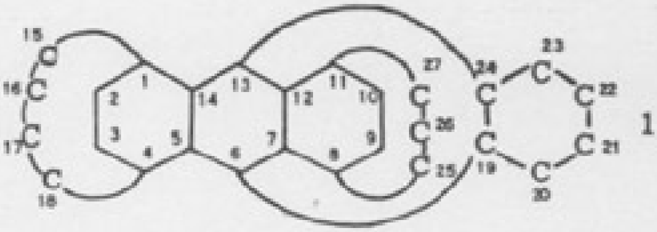
1b.

(3)



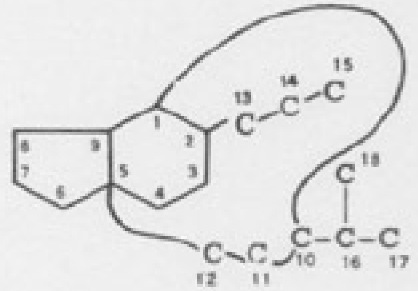
1.c.

(4)



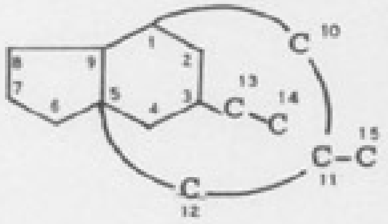
1c.

(5)



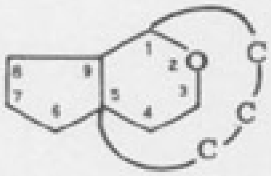
2b(2)

(6)



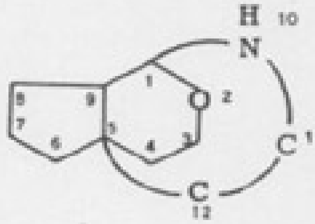
2b(1)

(7)



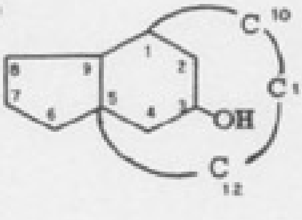
2.61-1

(8)



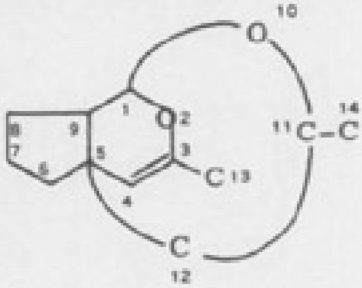
2.61-1.

(9)



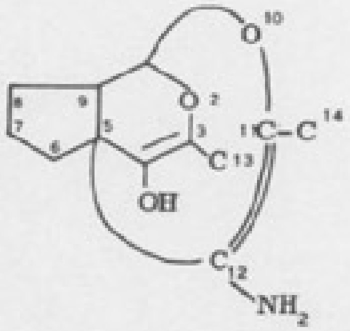
2.61-2a.

(10)



2.61-2c.

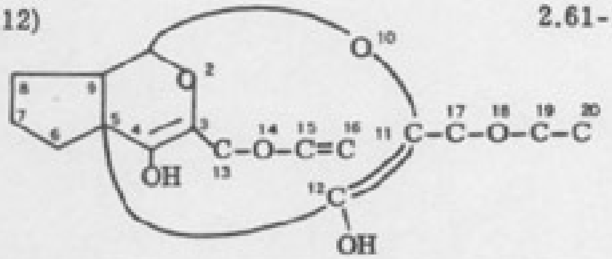
(11)



2.61-2b.

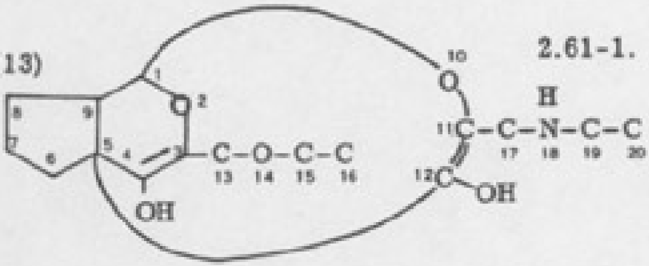
(12)

2.61-1.

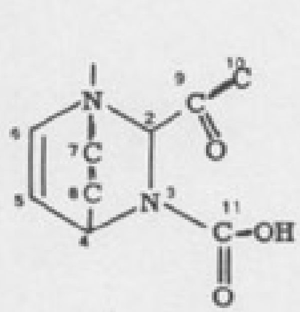


(13)

2.61-1.



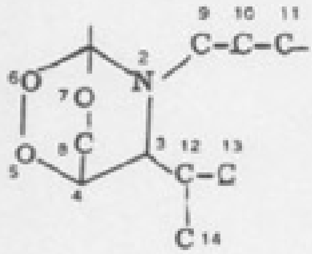
(14)



6.7-2b(1)

6n*LL(1)L(CVM)n(CVQ)L(1)L:L

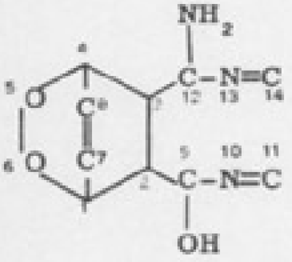
(15)



6.7-2b(2)

6L*OL(1)n(C3)LTL(1)OO

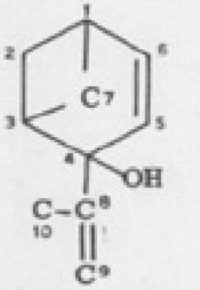
(16)



2.61-2b.

6L*L:L(1)L(CQN=C)L(CZN=C)L(1)OO

(17)

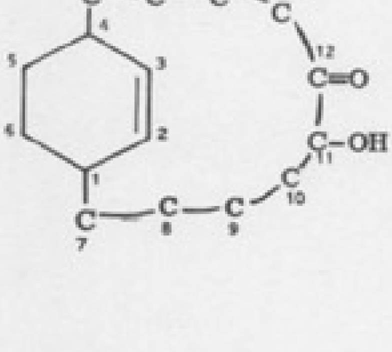


6.7-2a.

6L*L(1)LL(1)LQ(CM=C)L:L

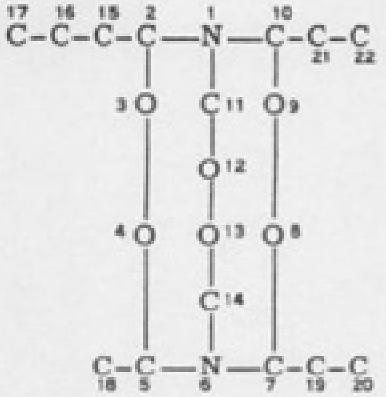
2.61-2b.

(18)



6L*L4LQLVL4(1)L:LL(1)LL

(19)



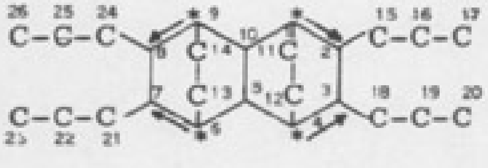
6.7-2b(1)

1Δn*LOOL(1)L(C3)OOLMn(1)LEOOLE

The following examples show how the enumeration pattern of a symmetrical bridged ring hydrocarbon accommodates derived features:

Parent hydrocarbon:

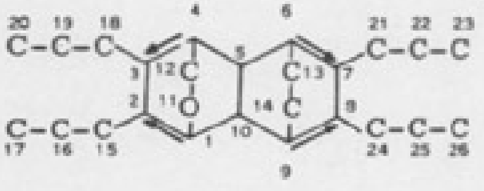
(20)



Derivatives (starting atom selected by Sec. 6.7, feature 3):

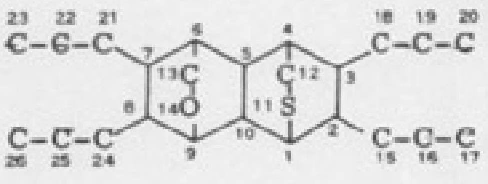
2.61-1

(21)

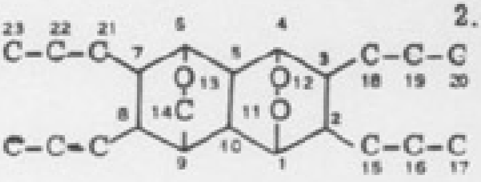


2.61-1

(22)

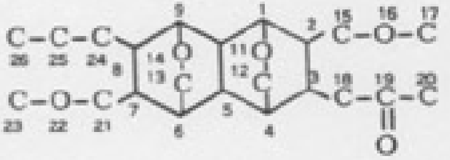


(23)



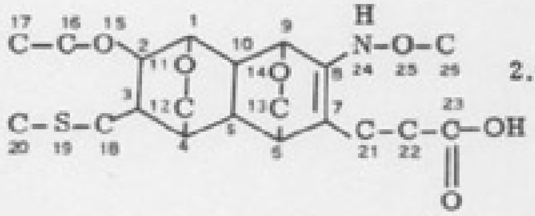
2.61-1

(24)



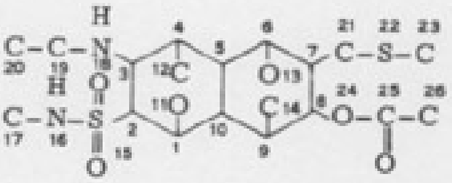
2.61-1

(25)



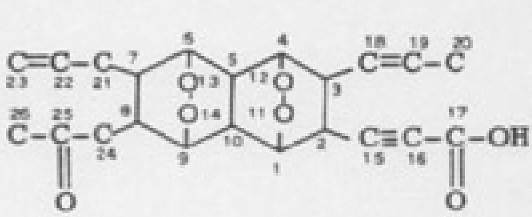
2.61-1

(26)



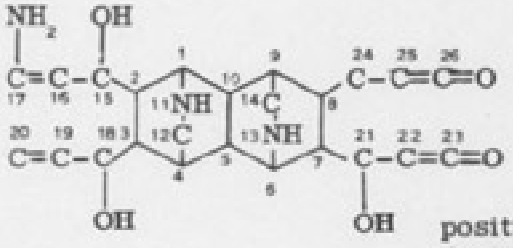
-1

(27)



-2a.

(28)

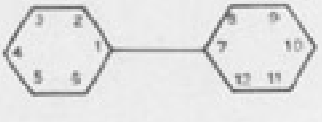


-2a
position 18
decisive

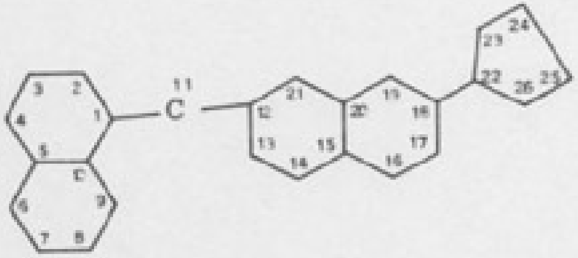
A molecule which contains more than one discrete ring system is classified as a ring assembly whether or not the systems are connected together by bonds only or by atoms in addition. The ring systems included may be single rings or fused ring aggregates, bridged or unbridged. A ring assembly may be random, wherein all of the linkages between component ring systems are acyclic, or circular, wherein at least two of the component ring systems are connected by atoms and/or bonds external to each so as to form a closed circular path which includes at least three atoms of each of the two last mentioned component systems. A circular ring assembly may include a plurality of circular paths of the type just described and in addition may include component systems which are random with respect to each other. The enumeration, as illustrated by the following formulas, will be explained in later sections.

EXAMPLES of ring assemblies:

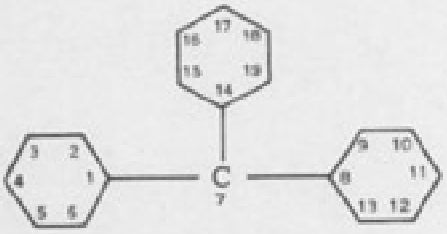
(1)



(2)



(3)



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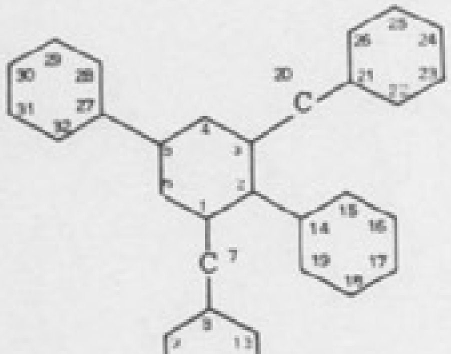

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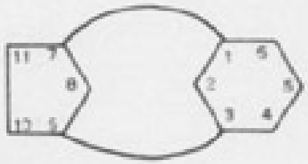
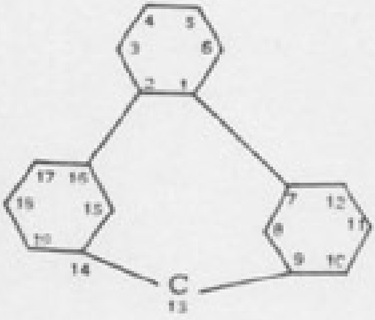
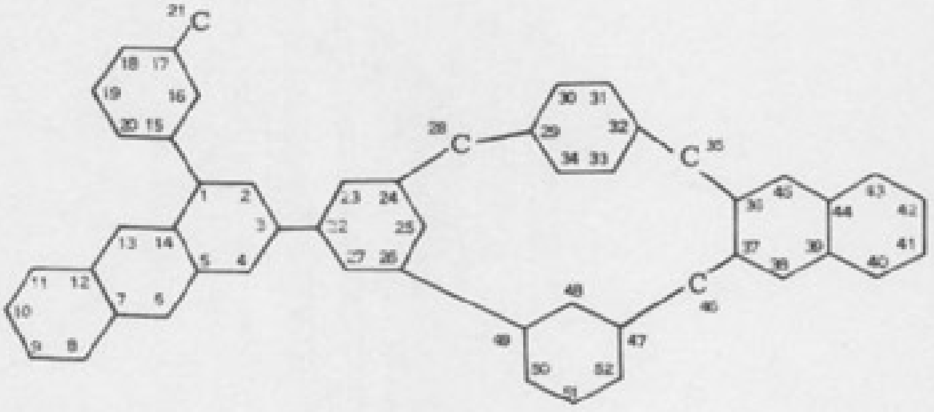


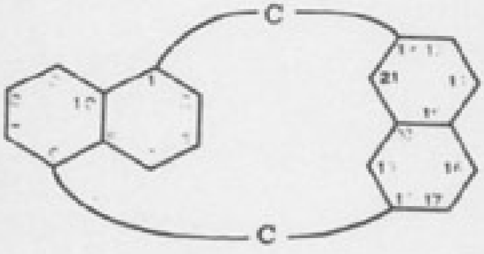
(6)



(7)



(8)



7.1 THE PLANAR DIAGRAM OF A RING ASSEMBLY

In the planar diagram of a ring assembly each component system must be expressed in its systematic planar configuration when the system is bridged, as described in Sec. 6.4. The atoms and/or bonds which connect the component systems of a circular assembly are treated as acyclic and ciphered by acyclic symbols.

7.2 ORDER OF ENUMERATION OF A RING ASSEMBLY

The configurations of a ring assembly are enumerated sequentially in the following order of decreasing priority:

1. generating ring system (bridges included, if any) in the manner heretofore described for the particular class of ring system;
2. skeletal substituents attached to the generating ring system in the ascending numerical order of the generating system atoms to which such groups are attached and in the order described in Section 7.4 when a plurality of skeletal substituents are attached by acyclic bonding to the same atom.

7.21 Enumerate component ring systems and skeletal substituents thereof in the same order as that described for the generating ring system. Enumerate around each newly introduced component ring system in the direction prescribed by Section 7.3.

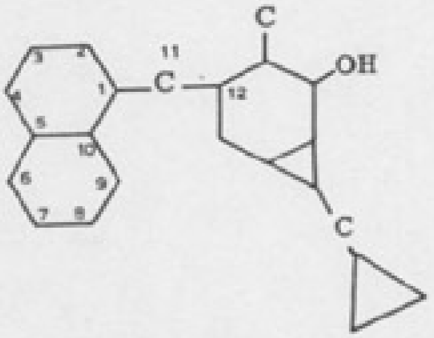
7.3 DIRECTION OF ENUMERATION AROUND A RING SYSTEM WHICH DOES NOT CONTAIN THE STARTING ATOM

Any component ring system which does not contain the starting atom for the enumeration of the assembly bears a substituent relationship to the next lower numbered ring system to which it is directly, or indirectly, attached.

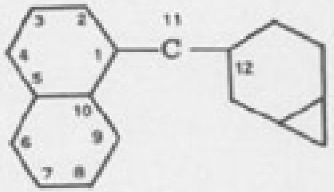
After enumerating the first atom of a substituent ring system continue to enumerate around the system in that peripheral direction which generates, in accordance with Section 4.1 or 5.2-5.3 depending upon whether the ring system concerned is a single ring or a fused ring aggregate, the ascending enumeration pattern which assigns the lower number on the occasion of the first difference, to the structural features listed in Section 6.7 in their same order of priority.

The state of the component system to which feature 1a. of Section 6.7 applies is that in which all substituents and bridges, if any, have been replaced by the necessary hydrogen atoms. The already enumerated portion of the molecule is not a substituent of the newly introduced system and remains attached.

EXAMPLE:

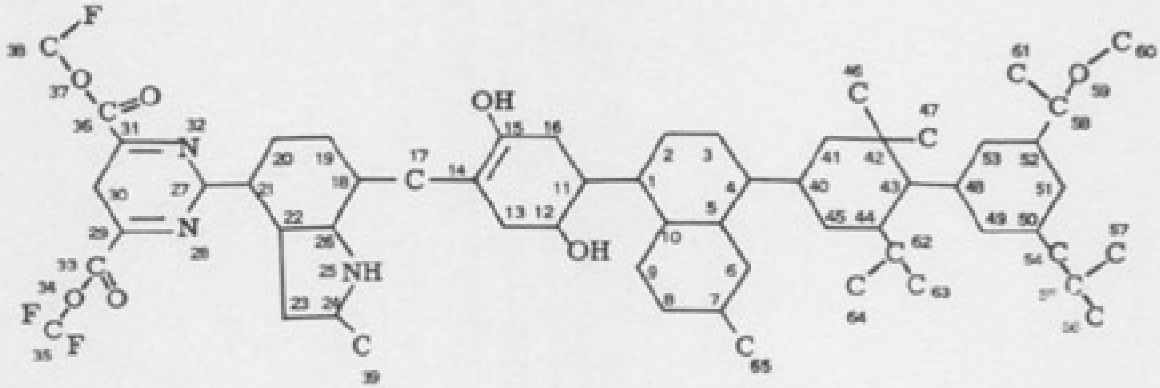


normal state of
"12" system



bridge and substituent free
state of "12" system

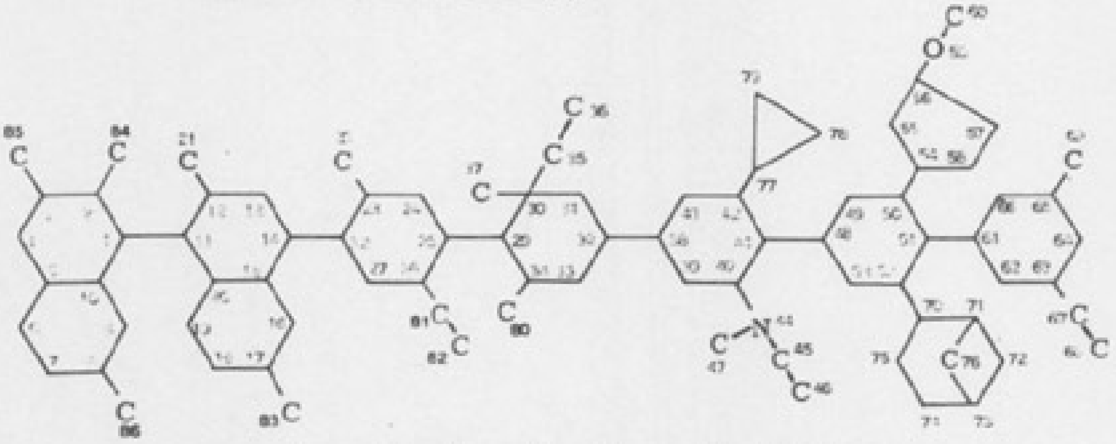
(1)



Direction of enumeration from atom	Decided by Section 6.7 feature
1	2a. (at atom 7)
11	3; 2.61-2a. (at atom 12)
18	1a. (at atom 19)
27	3; 2.61-2a. (at atom 35)
40	2a. (at atom 42)
48	2b(2) (at atom 54)

See also 7.5 EXAMPLE (1).

(2)



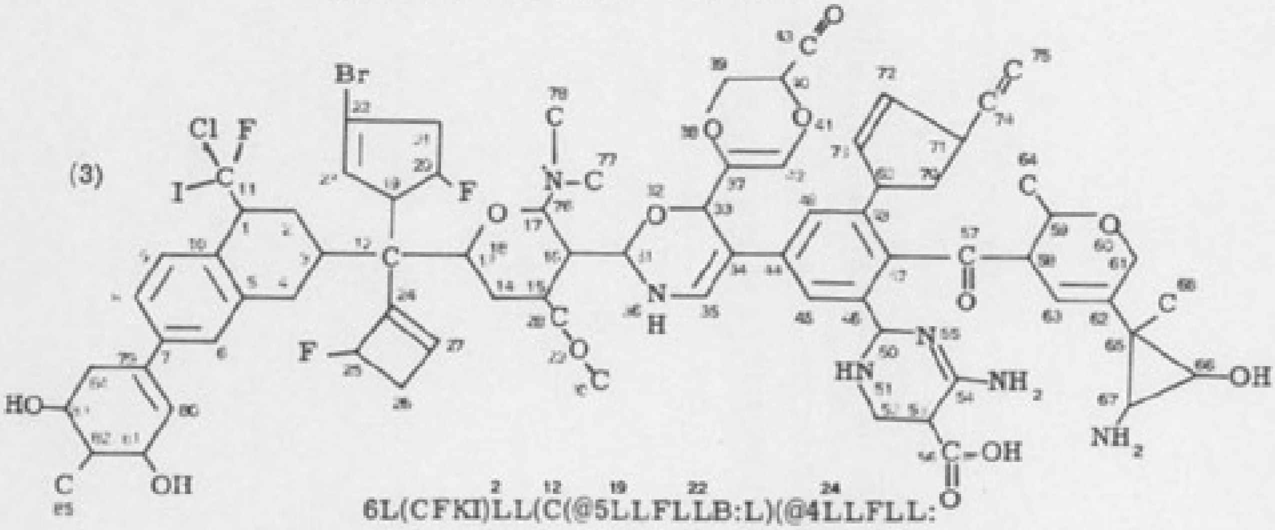
```
    11  14  22  25  29   32 38 40
6L(@6LLMLL(@6LLMLL(@6LLEMLL(@6LLL

    41 48 50  54     58 51  61
(NME)L(@6LLL(@5LLL(OM)LL)L(@6LLLELL

66 52  71 76  73  74 75 53 42   49
ML)L(@6LL*L(1)LL(1)LL)L)L(@3LLL)L)LLM)

26 15    20  5     10
LEL)YLLMLLY)LMLMLYLLLMLY
```

(3)



```
        2 12  19  22      24
6L(CFKI)LL(C(@5LLFLLB:L)(@4LLFLL:

    13      16  31 33 37 40
)@6LLL(COM)L(@6LOL(@6LOLL(CV)O

  34  44 46  50  53    54   47 57
L:)L(@6RRR(@6LnHLL(CVQ)LZ:n)R(GV@

 58 60 62       67  63 48 69 71
6LLMOLL(@3LMLQLZ):L)R(@5LLL(C=C)

 73 49 35 17 76 18 4 5 7 79
L:L)R):LnH)L(NM2)O)LYRR(@6L:LLQLM

 84 8 10
LQL)RRY
```

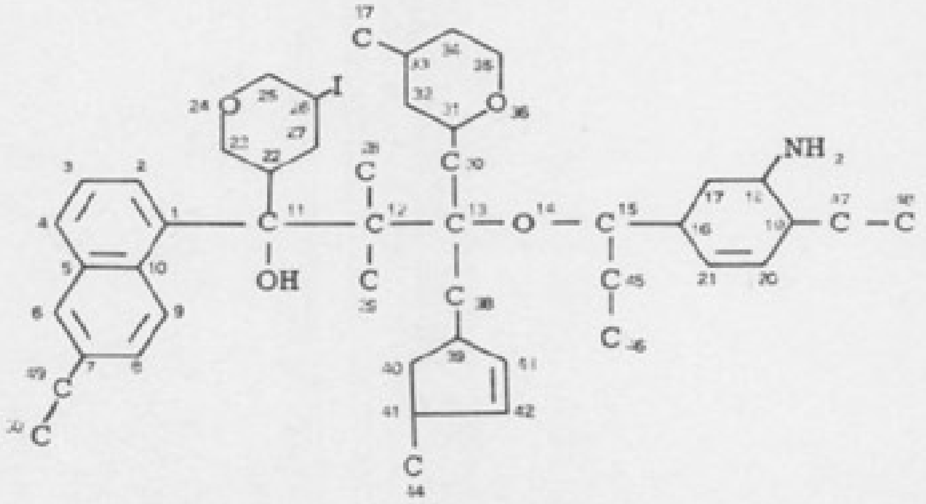
7.31 Order of Ascending Enumeration of the Branches of a Connecting Chain of a Ring Assembly

A. Enumerate skeletal paths which branch from the same enumerated atom of a connecting chain in the order in which they exhibit the following features listed in their order of decreasing priority:

1. greater number of skeletal atoms;
2. ascending enumeration pattern which assigns the lower number on the occasion of the first difference to the
   - a. carbon atom which bears the greater number of hydrogen atoms in the saturated hydrocarbon state of the path;
   - b. features listed in Section 2.61 in their same order of priority.

B. When an enumerated connecting chain, or branch thereof, terminates in a component ring system, enumerate around such system in the manner prescribed by 7.3. When the last atom of the component ring system has been enumerated, the atom(s) of the connecting chain, if any, and of the component ring system which establish an unbroken ascending numerical sequence constitute a substituent main path. Enumerate all unenumerated skeletal groups which are bonded to a substituent main path of the type just described in the ascending numerical order of the atoms of such path to which such groups are bonded.

EXAMPLE:



7.4 SELECTION OF THE GENERATING RING SYSTEM

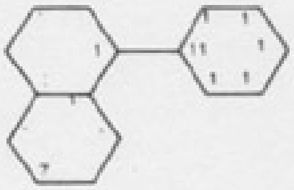
Select as the generating system (expressed in systematic planar form, if bridged) that component system which exhibits the following features listed in their order of decreasing priority:

1. greater number of
   - a. fused rings
   - b. ortho fused faces
   - c. six-membered rings
   - d. ring atoms (bridge atoms, if any, included)
2. ascending enumeration pattern which assigns the lower number on the occasion of the first difference to the features described in Sec. 6.7 in their same order of priority.

In the following examples the decisive feature of this Section which determines the selection of each generating system is indicated by its antecedent heading:

1. Greater number of fused rings (1a):

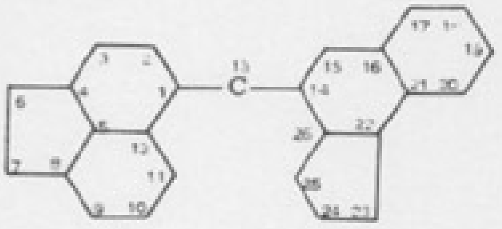
(1)



6L(@6LL5)L3YL4Y

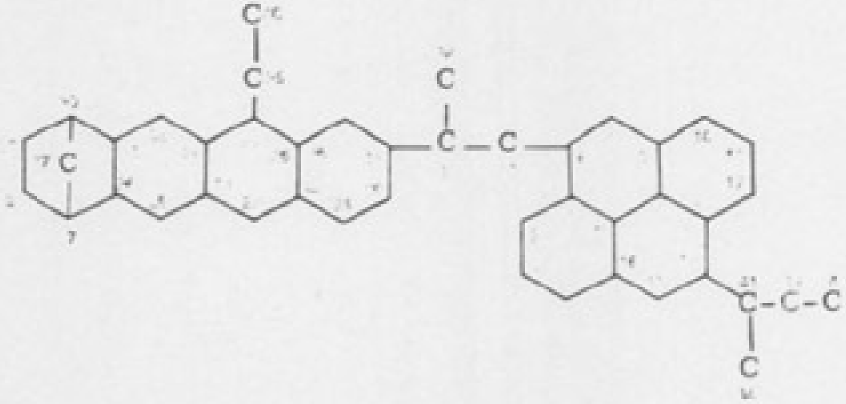
1. Greater number of ortho fused faces (1b.):

(2)



6L(C@6$\overset{14}{\text{L}}$LYL4YY5L3Y)$\overset{2}{\text{L}}$LY5y$\overset{6}{\text{L}}$LYL3Y

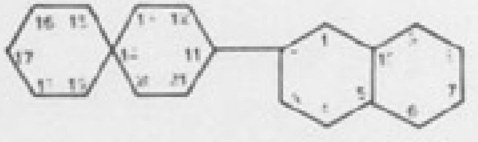
(3)



6L3Y$\overset{5}{\mathrm{y}}$L(CCM@6LLL$\overset{22}{\mathrm{Y}}$LYL$\overset{26}{\mathrm{Y}}$L*L(1)LLL(1)$\overset{31}{\mathrm{Y}}$LYLEY

L)$\overset{7}{\mathrm{L}}$Y$\overset{9}{\mathrm{y}}$L3Y$\overset{14}{\mathrm{L}}$(CME)LY

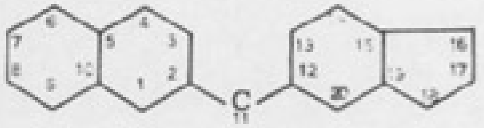
(4)



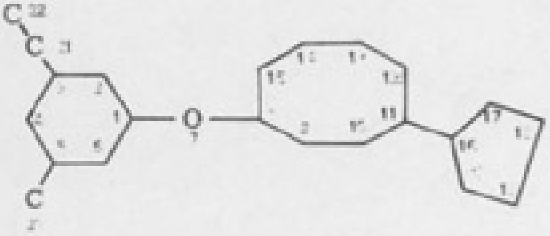
6L$\overset{2}{\mathrm{L}}$(@6$\overset{11}{\mathrm{L}}$LL$\overset{14}{\mathrm{X}}$L5-LL)$\overset{3}{\mathrm{L}}$LYL4Y

1. Greater number of six-membered rings (1c.):

(5)



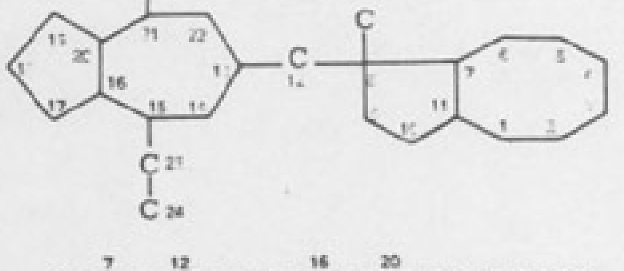
(6)



6L(O@8$\overset{8}{\mathrm{L}}$LLL(@$\overset{16}{\mathrm{5}}$LL4)L4)$\overset{2}{\mathrm{L}}$LELLML

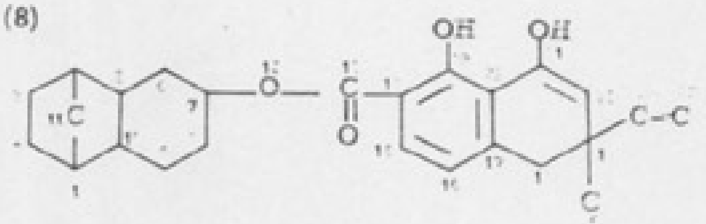
1. Greater number or ring atoms (1d.):

(7)



8L6$\overset{7}{\mathrm{Y}}$5L($\overset{12}{\mathrm{C}}$@7LLLE$\overset{16}{\mathrm{Y}}$5L3$\overset{20}{\mathrm{Y}}$7LML)MLLY8

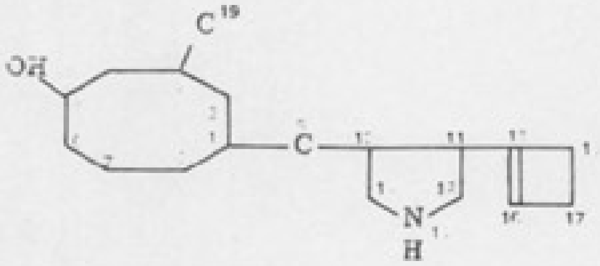
(8)



6L*$\overset{11}{\mathrm{L}}$(1)LL$\overset{4}{\mathrm{L}}$(1)YL$\overset{7}{\mathrm{L}}$(OCV@6RR$\overset{14}{\mathrm{R}}$$\overset{17}{\mathrm{Y}}$LLEML:LQYRQ)

$\overset{8}{\mathrm{L}}$LY

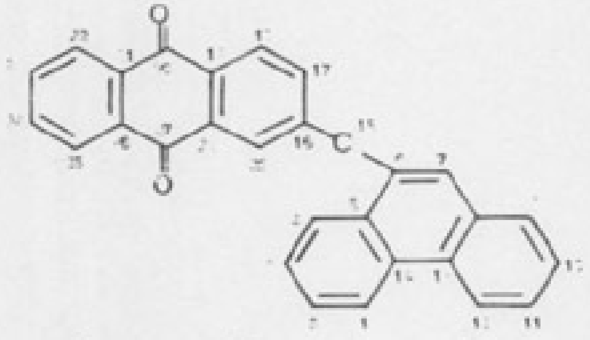
(9)



8L(C@5L$\overset{11}{\mathrm{L}}$(@4L:LLL)$\overset{12}{\mathrm{L}}$nHL)$\overset{2}{\mathrm{L}}$LMLLQL3

2. Ring system path first richer in hydrogen in the saturated hydrocarbon state (6.7-1a.);

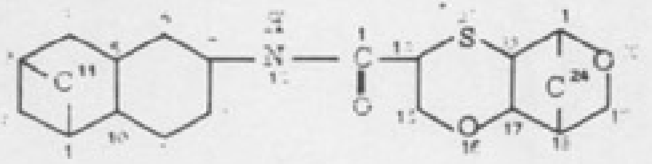
(10)



6R4Y$\overset{6}{\mathrm{R}}$(C@6RRRY$\overset{20}{\mathrm{L}}$VYR4YLVYR)$\overset{7}{\mathrm{R}}$YR4YY

2. Greater number of bridges (6.7-1b.):

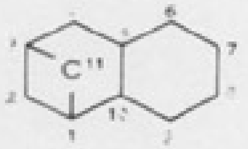
(11)

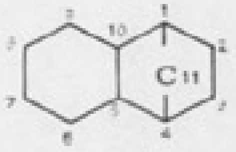


$$\mathrm{6L{*}\overset{11}{L}(1)L\overset{3}{L}(1)LYL\overset{7}{L}(NHCV@6LLOYL{*}\overset{24}{L}(2)}$$

$$\mathrm{LOL(2)YS)\overset{8}{L}LY}$$

Saturated hydrocarbon states of above bridged systems:



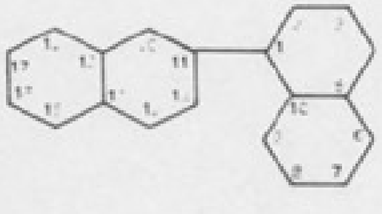


2. Greater number of skeletal substituents (6.7-2a.):

(12)

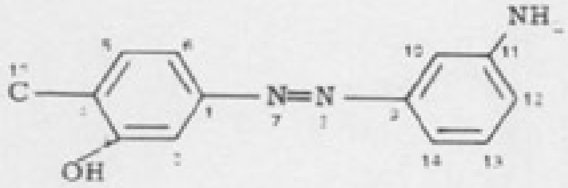
$$\mathrm{6L(SWNH@6\overset{8}{L}LLML3)\overset{2}{L}ML4}$$

(13)



$$\mathrm{6L(@6\overset{11}{L}LLYL4YL)\overset{2}{L}3YL4Y}$$

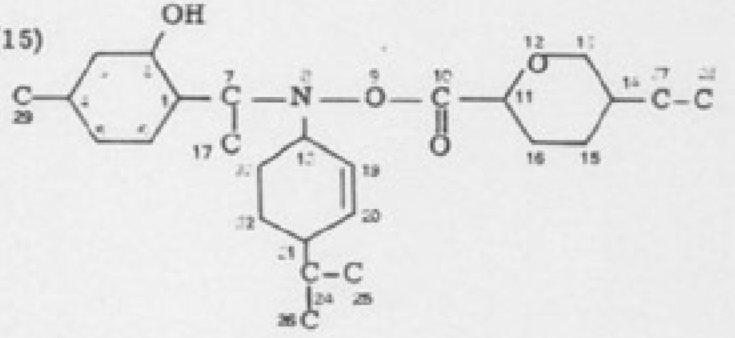
(14)



$$\mathrm{6R(N{=}N@6RRRZR3)\overset{2}{R}RQ\overset{4}{R}MRR}$$

2. Skeletal substituent having greater number of skeletal atoms (6.7-2b(1)):

(15)



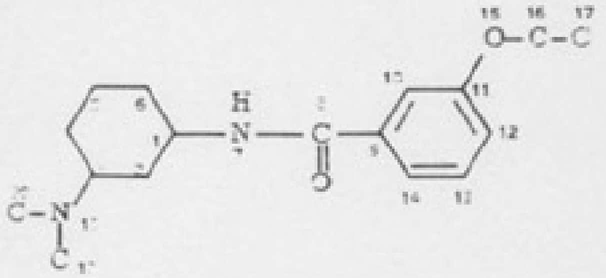
$$\mathrm{6L(CMN(@6\overset{18}{L}L{:}LLTLL)\overset{9}{O}CV@6\overset{12}{L}OL\overset{14}{L}ELL)}$$

$$\mathrm{\overset{2}{L}QL\overset{4}{L}MLL}$$

In the above assembly the "winning" substituent is constitued by atoms 7-28, which has one more skeletal atom than the substituent of atom "11" and two more than the substituent of atom "18". The substituent of atom "11" is constituted by all atoms except atoms 11-16 and 27-28; the substituent of atom 18, by all atoms except atoms 18-26.

2. Ascending enumeration pattern of saturated hydrocarbon state of substituent (6.7-2b(2)):

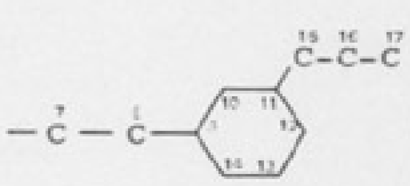
(16)



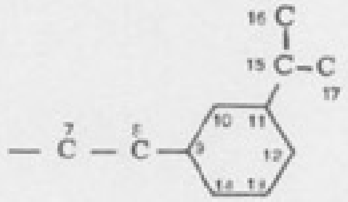
$$\mathrm{6L(NHCV@6\overset{9}{R}RRR(OE)\overset{12}{R}3)\overset{2}{L}\overset{3}{L}(NM2)L3}$$

The contending substituents are the ones attached to atoms "1" and "9" both of which have the same number of skeletal atoms, namely eleven. The saturated hydrocarbon states of the two substituents are as follows:

atom "1" subst:



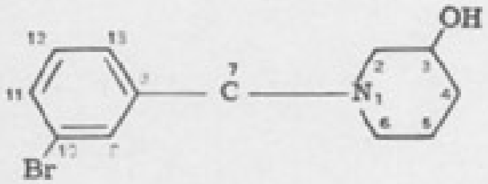
atom "9" subst:



The required order of ascending enumeration of the substituents, as shown, indicates that the "15" position of the atom "1" substituent bears a greater number of hydrogen atoms than the competing "15" position of the atom "9" (compound formula) substituent. Accordingly atom "1" must begin the enumeration as shown in the above structural formula.

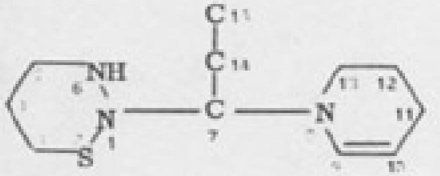
2. Heavier skeletal atom (2.61-1):

(17)



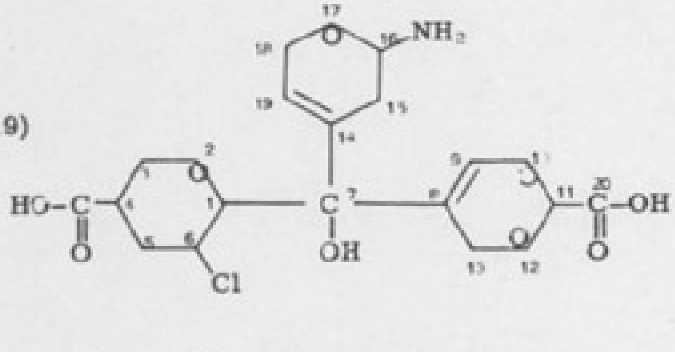
6n($\overset{7}{\text{C}}$@6$\overset{8}{\text{R}}$RRRBR3)$\overset{2}{\text{L}}$LQLLL

(18)



6n(CE@6nL:LLLL)SLLLnH

(19)

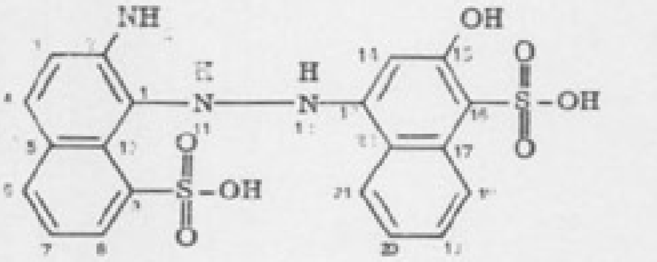


6L($\overset{7}{\text{C}}$Q(@6$\overset{14}{\text{L}}$LLZOLL:)@6$\overset{8}{\text{L}}$:LOL(CVQ)OL)

$\overset{2}{\text{O}}$L$\overset{4}{\text{L}}$(CVQ)L$\overset{6}{\text{L}}$K

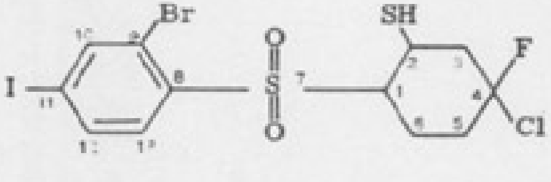
2. Greater number of functional substituents (2.61-2a.):

(20)



6R(NHNH@6$\overset{13}{\text{R}}$RRQ$\overset{16}{\text{R}}$(SWQ)YR4Y)$\overset{2}{\text{R}}$ZRRYR3$\overset{9}{\text{R}}$(SWQ)Y

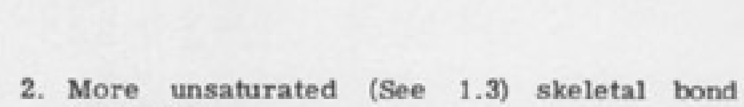
(21)



6L($\overset{7}{\text{S}}$W@6RR$\overset{9}{\text{B}}$RR$\overset{11}{\text{I}}$RR)$\overset{2}{\text{L}}$(SH)LL$\overset{4}{\text{F}}$KLL

2. Heavier functional substituent (2.61-2b.):

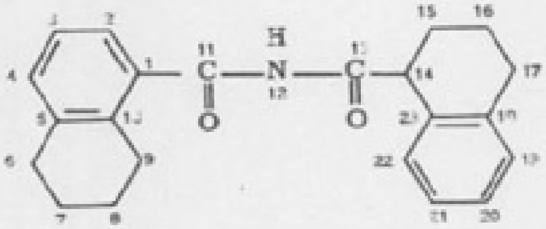
(22)



6L($\overset{7}{\text{C}}$VCQ$\overset{9}{\text{C}}$ZCV@6$\overset{11}{\text{L}}$OL$\overset{14}{\text{L}}$(CVM)LL)$\overset{2}{\text{O}}$LL(CVM)LL

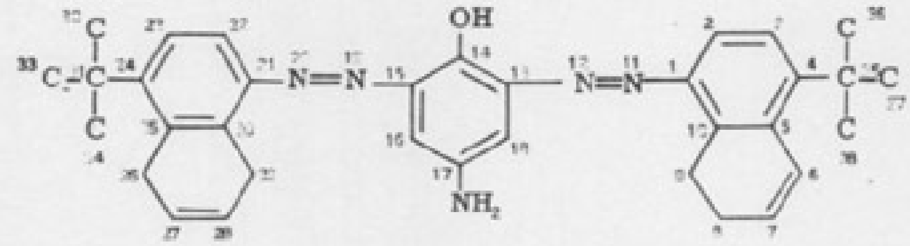
2. More unsaturated (See 1.3) skeletal bond (2.61-2c.):

(23)



6R(CV$\overset{12}{\text{N}}$HCV@6$\overset{14}{\text{L}}$L3Y$\overset{18}{\text{R}}$4Y)$\overset{2}{\text{R}}$3YL4Y

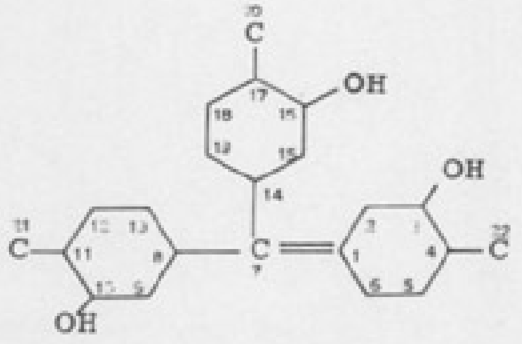
(24)



$\mathrm{6R(\overset{11}{N}{=}N@6R\overset{14}{R}Q\overset{15}{R}(N{=}N@6\overset{21}{R}RR\overset{24}{R}(CM3)YLL{:}LL\overset{30}{Y})}$

$\mathrm{\overset{16}{R}RZ\overset{18}{R})\overset{2}{R}R\overset{4}{R}(CM3)\overset{5}{Y}L{:}LLLY}$

(25)



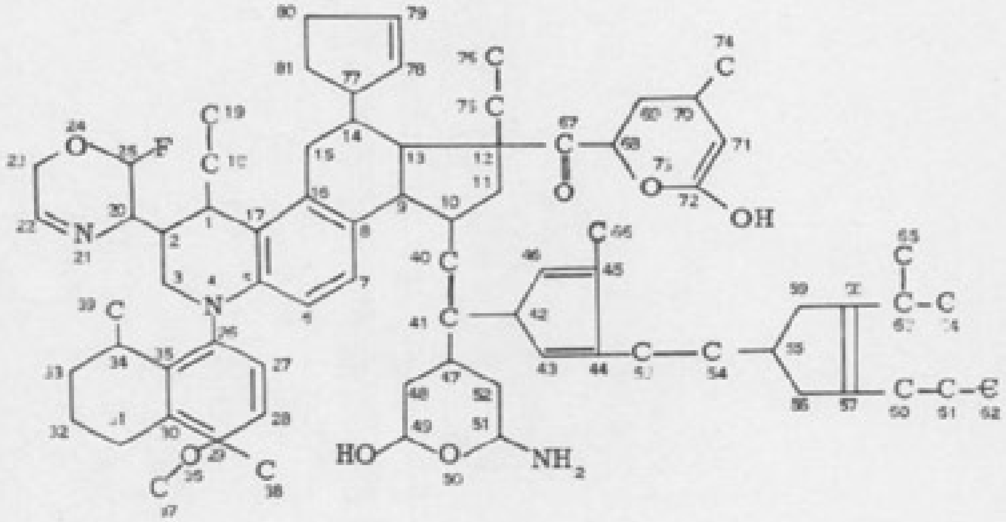
$\mathrm{6L(=C(@6LLLQLMLL)\overset{*}{2}\overset{2}{L}LQLMLL}$ * See 2.8-4.

7.5 ENUMERATION PATTERN, STARTING ATOM AND PERIPHERAL DIRECTION FOR ENUMERATION OF THE GENERATING RING SYSTEM

Begin the enumeration with that atom of the generating ring system and continue to enumerate in that peripheral direction which generates the ascending enumeration pattern which assigns the lower number on the occasion of the first difference to the features listed in Sec. 6.7 in their same order of priority.

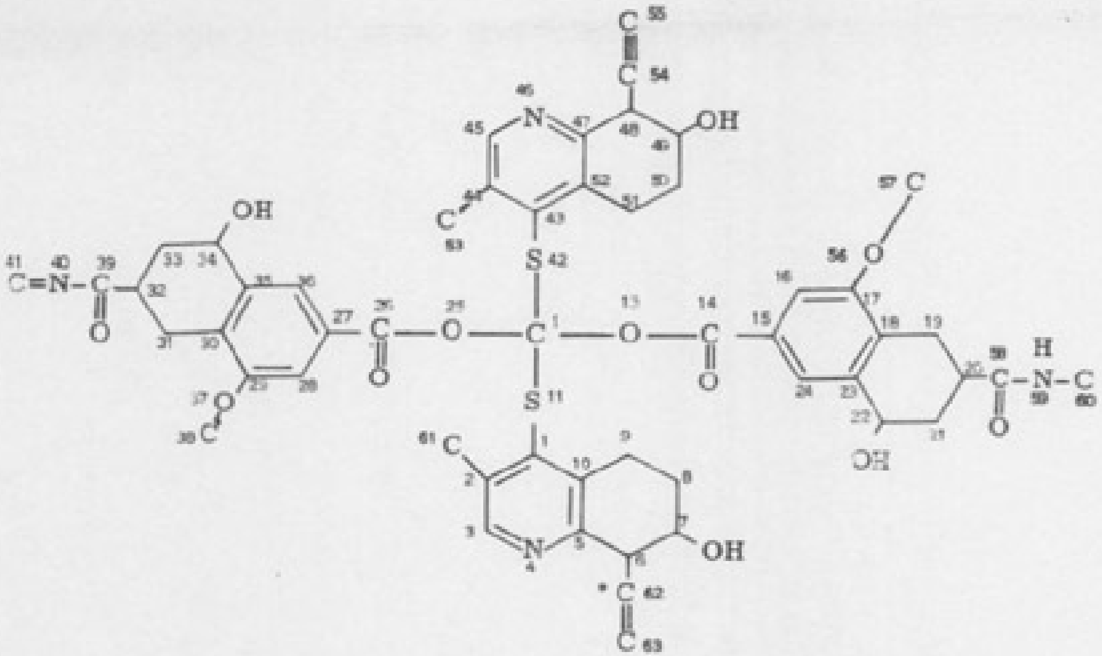
EXAMPLES:

(1)



Ascending enumeration order from atom:	Decided by feature:
1	6.7 - 1a.
20	6.7 - 3; 2.61-1 at atom 21
26	6.7 - 1a.
41	7.31-1.
42	6.7 - 2b(1) at atom 44
47	6.7 - 3; 2.61-2b.
55	6.7 - 2b(2).
68	6.7 - 2a.
77	6.7 - 3; 2.61-2c.

(2)



*decisive position for selection of the generating system

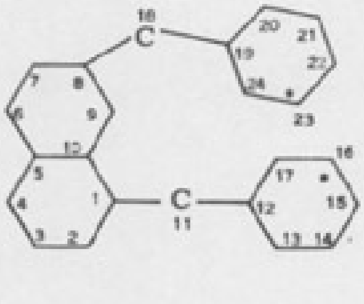
cipher: 6R(S$\overset{12}{C}$(OCV@6RR$\overset{24}{R}$(OM)YL$\overset{32}{L}$(CVN=C)L$\overset{34}{L}$Q$\overset{35}{Y}$R)(S@6RMR$\overset{46}{n}$Y$\overset{49}{L}$(C+C)LQLLY)$\overset{13}{O}$CV@6$\overset{18}{R}$R
$\overset{17}{R}$(OM)YLL(CVNHM)LLQYR)$\overset{2}{R}$MR$\overset{4}{n}$YL(C=C)LQLLY

7.6 CIRCULAR RING ASSEMBLIES. ORIENTATION

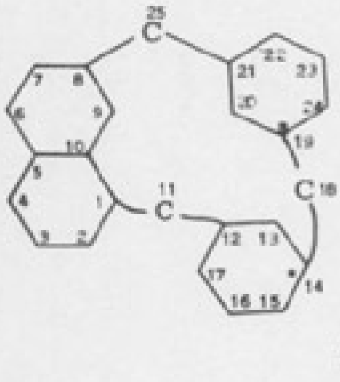
A circular assembly is viewed as a random assembly in which two or more of the component ring systems are hooked together by an extraneous bond or polyvalent radical so as to form a closed path. All of the component ring systems which are included in the circular path are considered to lie in the same reference plane, and any component system which is bridged must be represented in its systematic planar form (see Section 6.) for purposes of enumeration, just as in the case of random assemblies.

In the following examples the atoms of the two component systems of each random assembly which are linked together to form the corresponding circular assembly are labelled by asterisks.

Random:

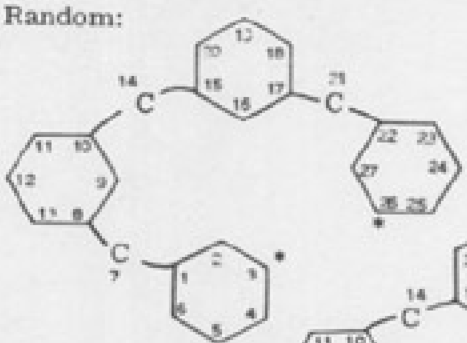


Circular:

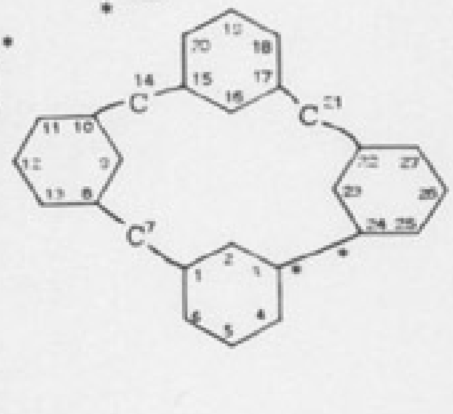


NOTE: All component ring systems and connecting links which lie outside of the generating ring system are considered to be a substituent of the lower numbered atom of the generating system to which such substituent is bonded. In the above circular assembly atoms 11 to 25 constitute a substituent of atom 1. The enumeration patterns do not correspond because of difference in parent-substituent relationships occasioned by the head-to-tail hook-up. In the above case the substituent of atom 8 of the random assembly merges with the substituent of atom 1 of the circular assembly.

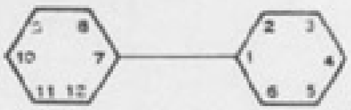
Random:



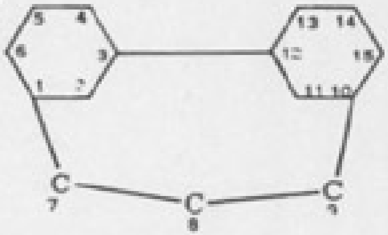
Circular:



Random:



Circular:

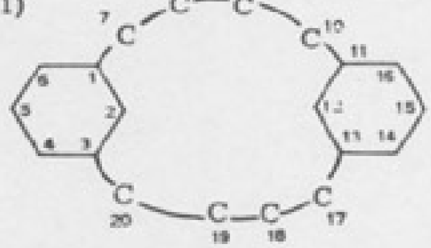


7.61 Definition of Circular Ring Assembly

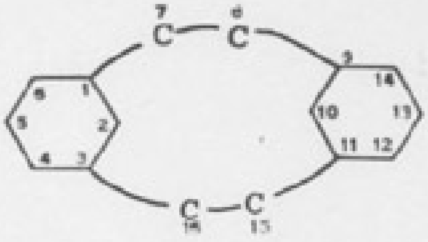
As stated above a circular assembly may be formed by linking together two component systems of a random assembly. Any molecule which contains a closed path of atoms and bonds which path is comprised of three or more atoms from each of two different rings, which two are not ortho- or spiro-fused to each other, is classified as a circular ring assembly. The examples immediately below illustrate molecules which possess the minimum structural requirement for classification as a circular assembly. Note that the number of atoms in the described path has no direct bearing on the classification, except that the minimum number is six by definition.

EXAMPLES:

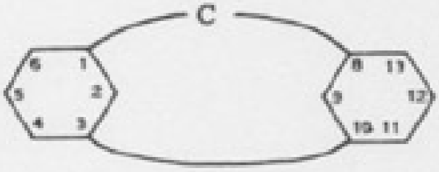
(1)



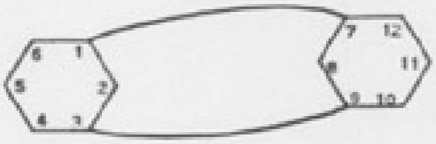
(2)



(3)



(4)

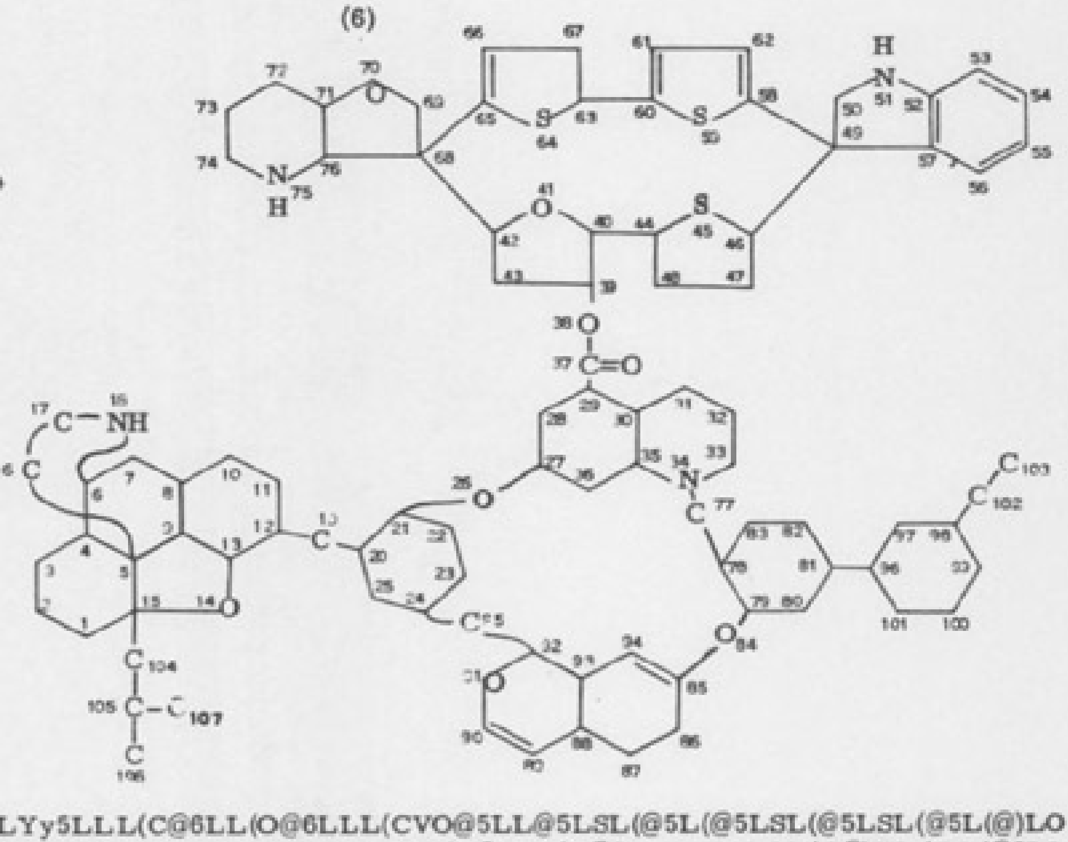


Aside from the minimum structural features required of two of the component ring systems of a circular assembly, there is no restriction placed on the number or kind of component ring systems which may comprise a circular assembly.

EXAMPLES:

(5)

(6)



cipher: 6L3Yy5*LLnH(1)L(1)LYy5LLL(C@6LL(O@6LLL(CVO@5LL@5LSL(@5L(@5LSL(@5LSL(@5L(@)LO YLLLnHY5):LL):LL:)LnHYR4Y5)LL)OL( )L)YLLLn(C@6LL(O@6LLLYL:LOL(C@)YL:)LL(@6LL LEL3)LL)YL)LLL( )L)Y5OY(CT)

Note that the linkages at atoms 49 and 68 are not enumerated as spiro since the connecting links of the closed circular path are considered acyclic. The enumeration is according to Sec. 7.3, feature 1.

7.615 EXAMPLES OF CIRCULAR ASSEMBLIES
Revised Ring Index numbers:

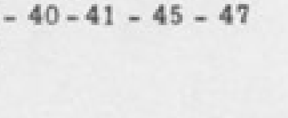
2132 - 34
2436
2580 - 84 - 86
2871 - 73
3185 - 97
3332
3777 - 78 - 81 - 84 - 86 - 92 - 94 - 97
3800 - 01 - 07 - 09 - 52
5341 - 43 - 45 to 50 - 52
5474 to 82
5616
5781 - 84 - 85
6123
6457 - 59 - 61 - 63 - 64 - 66 - 67 - 68 - 71 - 77
7053
7104 - 06 - 74 - 78
7404 - 10
7412 - 14
7536 - 37 - 40 - 41 - 45 - 47
7628 - 30
7702
7714

7.62 Structural Distinctions Among Fused Ring Aggregates, Bridged Ring Aggregates, and Circular Assemblies

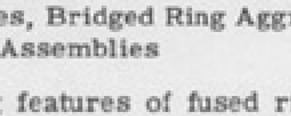
The defining features of fused ring aggregates and bridged ring aggregates are set forth in Sections 5. and 6., respectively; those of circular assemblies, in Section 7.61, preceding.

The following examples illustrate the structural feature which distinguishes circular ring assemblies from fused ring aggregates and bridged ring aggregates. Each "A" formula is a fused ring aggregate; each "B" formula, a bridged ring aggregate; and each "C" formula, a circular ring assembly.

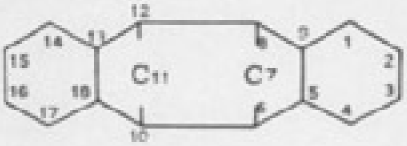
(1) A.



B.



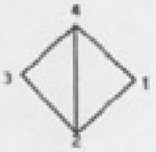
C.



In formula C the closed path is defined by atoms 6-8 and 10-12 and their connecting bonds. The two component ring systems are constituted by the two Indane systems, represented by atoms 1-9 and 10-18, which are joined to the closed path by other than ortho or spiro fusion and thereby form a circular assembly. In formula A all rings are joined by fusion (limited to ortho and spiro, as explained in Section 5.0) in the reference plane and is accordingly a fused ring aggregate. In formula B the rings formed by atoms 5, 6, 15, 13, and 14 and by atoms 6, 7, 12, 13, and 15 are not joined by ortho or spiro fusion and no closed path which includes atoms 6, 15, and 13 is joined by any other ring by other than ortho or spiro fusion; therefore formula B is not classified as a fused ring aggregate or as a circular assembly but as a bridged ring aggregate wherein atom 15 and its connecting bonds constitute the bridge, which is considered to lie in a different plane from the remaining ring atoms.

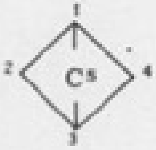
As illustrated below, the cipher of a fused ring aggregate never contains an asterisk "*" or the symbol "@"; the cipher of a bridged ring aggregate, always an asterisk but never an @; and the cipher of a circular (or random) assembly, always an @.

(2) A.



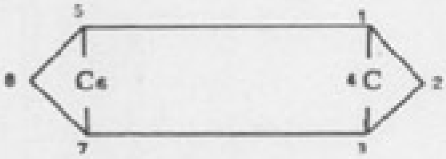
3LY3LY3

B.



4L*L(1)LL(1)L

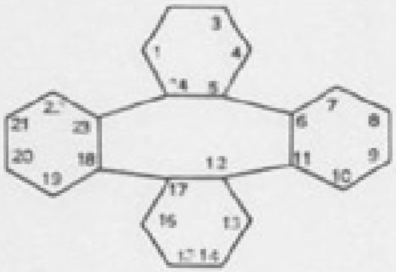
C.



4L(@4$\overset{5}{\text{L}}$LL(@L)$\overset{2}{\text{L}}$L( )L

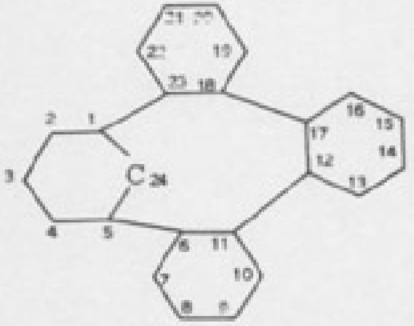
In formula C each four membered ring joins the closed path defined by atoms 1, 4, 3, 7, 8, 5 and their connecting bonds by other than ortho or spiro fusion and is therefore a component ring system of a circular assembly.

(3) A.



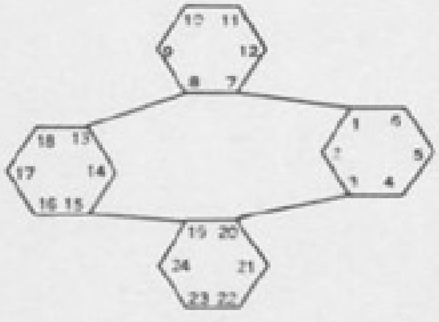
6L4Y8YL4Y8YL4Y8YL4Y8Y

B.



11L*L(1)L3L(1)YL4Y11YL4Y11YL4Y11

C.



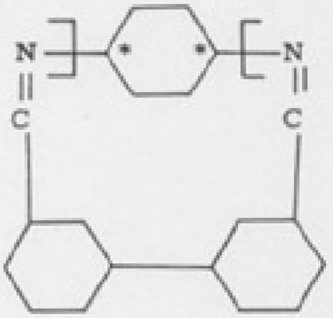
```
    7         13  15      19 20               2
6L(@6LL(@6LLL(@6LL(@)L4)L3)L4)LL( )L3
```

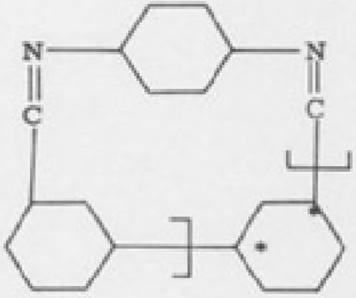
7.63 Parent-Substituent Relationships Among Skeletal Groups of a Circular Assembly

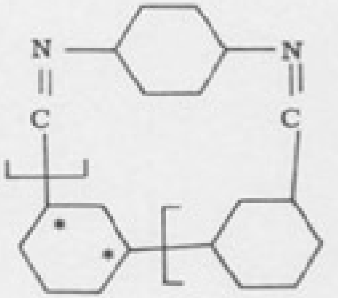
It is characteristic of a circular assembly that each component ring system which is included in the closed path is connected to such path by two bonds prior to enumeration. All of that portion of the molecule which is extraneous to each component system and is attached to it by the two connecting bonds is considered to be a substituent of each atom of the component system to which such extraneous portion is bonded. After the generating ring system and the starting atom for its enumeration have been selected, the above described extraneous portion becomes a substituent of the lowest numbered atom of the generating system to which such extraneous portion is bonded. All other parent-substituent relationships are the same as those described for random assemblies.

In the examples below that bracketed portion of each assembly is a substituent of each of the atoms marked by an asterisk:

EXAMPLES:







7.7 GENERATING RING SYSTEM OF A CIRCULAR RING ASSEMBLY

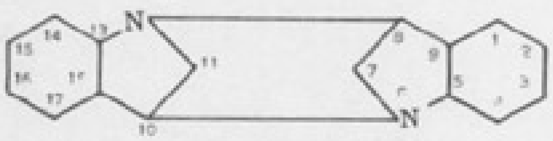
The procedure for the selection of the generating system is the same as that followed for the selection of the generating system of a random ring assembly; it being only necessary to keep in mind that in addition to regular substituents attached by acyclic bonds that portion of the molecule which lies outside of a given component ring system and comprises the circular assembly is a substituent of each atom of said ring system to which such outside portion is attached, as set forth in the previous section.

7.8 ENUMERATION. SPECIFIC PROCEDURE

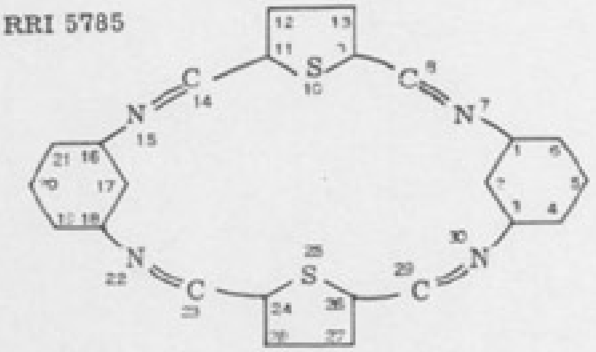
The definition of substituent as applied to the closed path of a circular assembly having been established, the enumeration of a circular assembly follows the same procedure as that set forth for the enumeration of a random ring assembly.

ENUMERATION EXAMPLES:

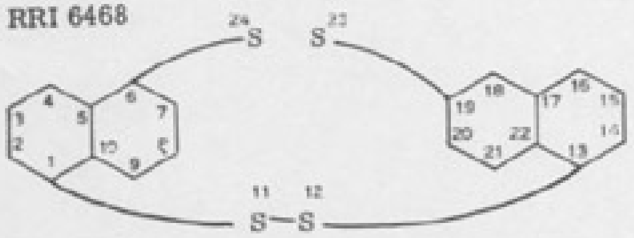
(1) RRI 5616



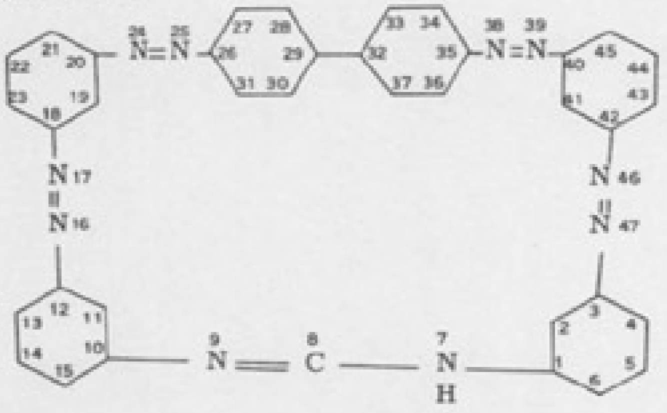
(2) RRI 5785



(3) RRI 6468



(4) RRI 7413



7.9 CIPHERING OF A CIRCULAR ASSEMBLY

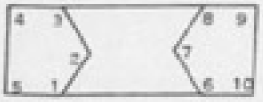
The procedure is the same as that used for ciphering a random assembly with the following modifications necessary to show the point of attachment of the "tail end" of the substituent portion of the assembly to the generating ring system:

1. After the cipher of the last configuration, which connects the "tail end" of the substituent portion to the generating system place the combination symbol "@)".

2. After the generating system atom to which the bond described in the preceding paragraph is attached place the combination symbol "( )".

All atoms and bonds which are not part of a component ring system but serve only to connect them are ciphered, not as ring atoms and bonds, but with the same symbols employed for connecting atoms and bonds of a random ring assembly.

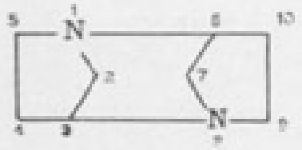
EXAMPLES (Ring Index Numbers Shown):



$$5L(@5\overset{6}{L}L\overset{8}{L}(@)\overset{0}{L}L)\overset{2}{L}\overset{3}{L}(\ )LL$$

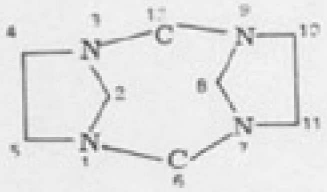
EXAMPLES (Revised Ring Index numbers shown in left margin):

(1) RRI 2438



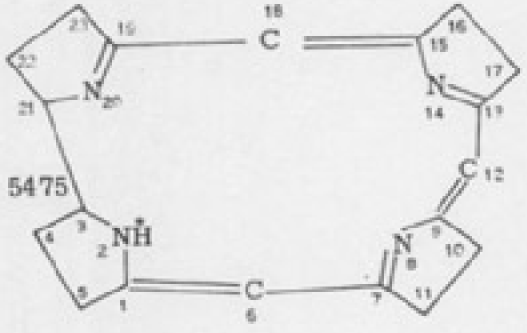
$$5n(@5\overset{6}{L}\overset{8}{n}(@)\overset{9}{L}L)\overset{2}{L}\overset{3}{L}(\ )LL$$

(2) RRI 2580



$$5\overset{1}{n}(C@5\overset{7}{n}Ln(C@)\overset{10}{L}L)\overset{2}{L}\overset{3}{n}(\ )L\overset{5}{L}$$

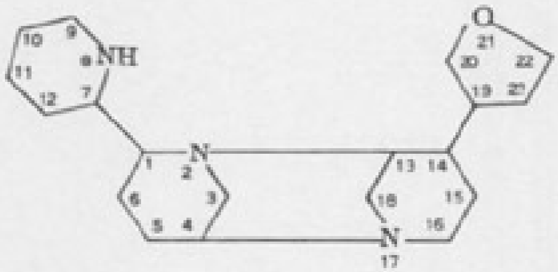
(3) RRI 5475



$$5L(=C@5\overset{7}{L}:nL(=C@5\overset{13}{L}:nL(=C@5\overset{19}{L}:n\overset{21}{L}(@)L\overset{23}{L})L\overset{17}{L})$$
$$L\overset{11}{L})\overset{2}{n}H\overset{3}{L}(\ )LL$$

*Ascending enumeration shown assigns the lower number (2.61) to the position "2" which bears the greater number of functional substituents—the H atom bonded to nitrogen "2".

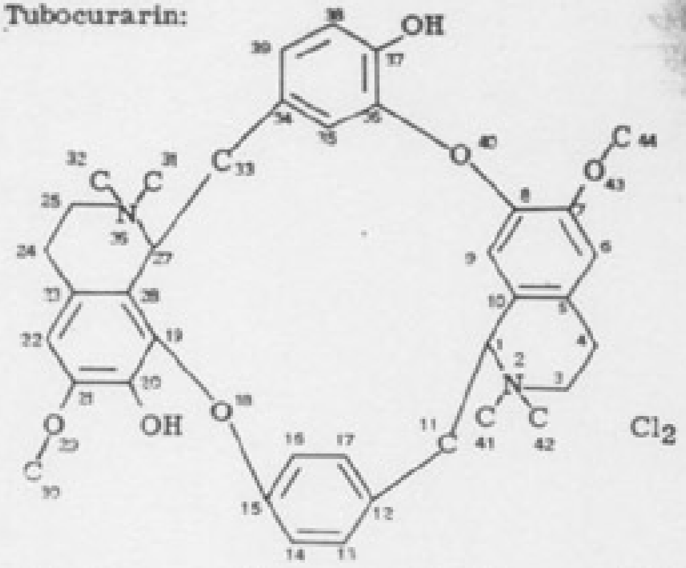
(4) RRI 2438



$\mathrm{6L(@6\overset{7}{L}nHLL3)\overset{2}{n}(@6\overset{13}{L}L(@5\overset{19}{L}LOLL)}$

$\mathrm{LLn(@)L)\overset{3}{L}L(\ \ )LL}$

(5) Tubocurarin:



$\mathrm{6L(\overset{11}{C}@6\overset{6}{R}RRRR(O@6\overset{19}{R}RRQR(OM)R\overset{23}{Y}LL\overset{26}{n}M2L(C@6\overset{34}{R}R\overset{36}{R}}$

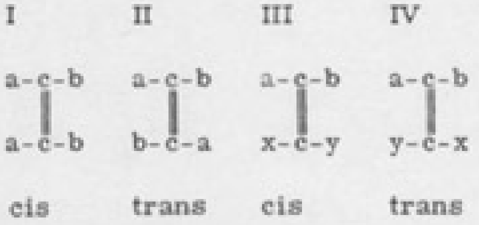
$\mathrm{(O@)\overset{37}{R}QR\overset{39}{R})\overset{28}{Y})\overset{16}{R}\overset{17}{R})\overset{2}{n}M2LL\overset{5}{Y}R\overset{7}{R}(OM)\overset{8}{R}(\ \ )R\overset{10}{Y}\ ;2[K]}$

Atoms "1" and "27" are closest contenders for starting atom. Atom 1 enumeration pattern assigns lower number "8" to ring atom which bears the greater number -one- of skeletal substituents on occasion of first difference.

8.0 STEREOISOMERS

8.01 CIS-TRANS ISOMERISM AT DOUBLE BONDS

The structural relationships necessary for cis-trans isomerism are represented schematically by formulas I, II, III, and IV below:



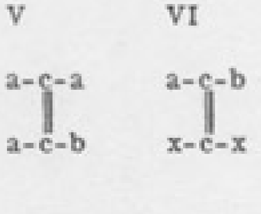
I $\begin{matrix}a\text{-}c\text{-}b\\ \|\\ a\text{-}c\text{-}b\end{matrix}$ cis

II $\begin{matrix}a\text{-}c\text{-}b\\ \|\\ b\text{-}c\text{-}a\end{matrix}$ trans

III $\begin{matrix}a\text{-}c\text{-}b\\ \|\\ x\text{-}c\text{-}y\end{matrix}$ cis

IV $\begin{matrix}a\text{-}c\text{-}b\\ \|\\ y\text{-}c\text{-}x\end{matrix}$ trans

The only requirement for geometric isomerism is that the substituents on each unsaturated atom are different. If either unsaturated atom carries two identical groups, then no isomerism exists. Formulas V and VI below display no isomerism



V $\begin{matrix}a\text{-}c\text{-}a\\ \|\\ a\text{-}c\text{-}b\end{matrix}$

VI $\begin{matrix}a\text{-}c\text{-}b\\ \|\\ x\text{-}c\text{-}x\end{matrix}$

8.02 ORIENTATION OF CIS-TRANS ISOMERS

Before deciding the cis-trans relationships in the manner described below, first establish the structural formulas so as to show the orientation of the groups about the double bond, or bonds, and enumerate the formula in the manner already set forth. For the sake of clarity the groups attached to unsaturated atoms should be oriented parallel to each other and perpendicular to the lines representing the double bond (Kekule), as shown in formulas I to IV, above—the groups must be on the same side in the formula representation as they are in the molecule represented.

8.03 DELINEATION OF CIS-TRANS CONFIGURATIONS AT ACYCLIC DOUBLE BONDS. SYMBOLS "(=)" AND "[=]"

The application of the designation cis or trans to the groups attached to the atoms joined by a double bond, as represented in formulas I to IV above, is decided with reference to

(1) the total number of enumerated groups attached to the double-bonded atoms
(2) the order of enumeration of such groups and/or

(3) the weight of such groups when neither group of a pair attached to the same double-bonded atom contains an enumerated atom.

It is possible for the double-bonded atoms to have a total of four, three, two, one, or no enumerated groups attached. Accordingly, the following five categories are treated below in the order given:

A. FOUR ENUMERATED GROUPS ATTACHED.
B. THREE ENUMERATED GROUPS ATTACHED.
C. TWO ENUMERATED GROUPS ATTACHED.
D. ONE ENUMERATED GROUP ATTACHED.
E. NO ENUMERATED GROUPS ATTACHED.

The term "pair," as used below under the above five headings, refers to the two groups attached to the same double-bonded atom.

In the cipher which appears below each related formula the double bond concerned is represented by the symbol (=) if the associated groups have a cis configuration and by the symbol [=] if the configuration is trans.

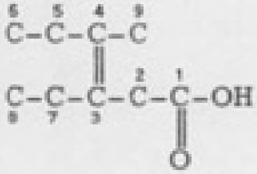
A. FOUR ENUMERATED GROUPS ATTACHED.

Cis—lower-numbered group of each pair on same side of double bond

trans—lower-numbered group of each pair on opposite side of double bond

EXAMPLES:

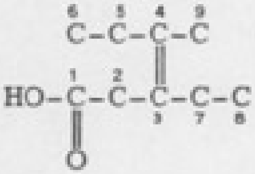
(1)



trans

CVQCCE[=]CME

(2)



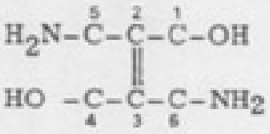
cis

CVQCCE(=)CME

(3)

3,4 configuration-trans; 6,7-cis
ECM[=]CMCCM(=)CME

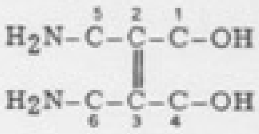
(4)



trans

CQC(CZ)[=]C(CZ)CQ

(5)



cis

CQC(CZ)(=)C(CZ)CQ

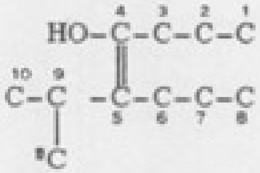
B. THREE ENUMERATED GROUPS ATTACHED.

cis—unenumerated group and lower-numbered group of enumerated pair on same side of double bond

trans—unenumerated group and lower-numbered group of enumerated pair on opposite side of double bond

EXAMPLES:

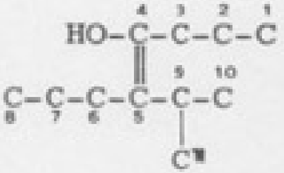
(6)



trans

C3CQ[=]CTC3

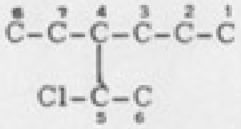
(7)



cis

C3CQ(=)CTC3

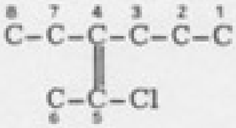
(8)



trans

C3CE[=]CKM

(9)



cis

C3CE(=)CKM

(10)

trans

MC[=]CME

(11)

cis

MC(=)CME

C. TWO ENUMERATED GROUPS ATTACHED.

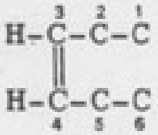
1. GROUPS ATTACHED TO DIFFERENT ATOMS.

cis—both enumerated groups on same side of double bond

trans-enumerated groups on opposite sides of double bond

EXAMPLES:

(12)

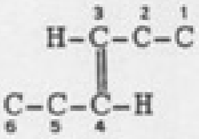


$$\begin{array}{ccccccc} H&-&\overset{3}{C}&-&\overset{2}{C}&-&\overset{1}{C}\\ &&\|&&&&\\ H&-&\underset{4}{C}&-&\underset{5}{C}&-&\underset{6}{C}\end{array}$$

cis

EC(=)CE

(13)

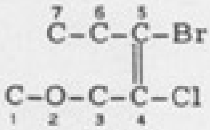


$$\begin{array}{ccccccccc} &&H&-&\overset{3}{C}&-&\overset{2}{C}&-&\overset{1}{C}\\ &&&&\|&&&&\\ \underset{6}{C}&-&\underset{5}{C}&-&\underset{4}{C}&-&H&&\end{array}$$

trans

EC[=]CE

(14)

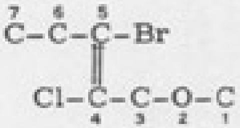


$$\begin{array}{ccccccccc} &&\overset{7}{C}&-&\overset{6}{C}&-&\overset{5}{C}&-&Br\\ &&&&&&\|&&\\ \underset{1}{C}&-&\underset{2}{O}&-&\underset{3}{C}&-&\underset{4}{C}&-&Cl\end{array}$$

cis

MOCCK(=)CBE

(15)



$$\begin{array}{ccccccccccc} \overset{7}{C}&-&\overset{6}{C}&-&\overset{5}{C}&-&Br&&&&\\ &&&&\|&&&&&&\\ &&Cl&-&\underset{4}{C}&-&\underset{3}{C}&-&\underset{2}{O}&-&\underset{1}{C}\end{array}$$

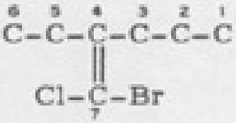
trans

MOCCK[=]CBE

2. BOTH ENUMERATED GROUPS ATTACHED TO SAME ATOM.
   cis—heavier unenumerated group and lower-numbered group on same side of double bond
   trans—heavier unenumerated group and lower-numbered group on opposite sides of double bond

EXAMPLES:

(16)

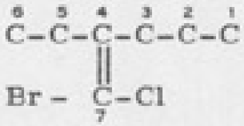


$$\begin{array}{ccccccccccc} \overset{6}{C}&-&\overset{5}{C}&-&\overset{4}{C}&-&\overset{3}{C}&-&\overset{2}{C}&-&\overset{1}{C}\\ &&&&\|&&&&&&\\ &&Cl&-&\underset{7}{C}&-&Br&&&&\end{array}$$

cis

C3C(=)CKB)E

(17)



$$\begin{array}{ccccccccccc} \overset{6}{C}&-&\overset{5}{C}&-&\overset{4}{C}&-&\overset{3}{C}&-&\overset{2}{C}&-&\overset{1}{C}\\ &&&&\|&&&&&&\\ &&Br&-&\underset{7}{C}&-&Cl&&&&\end{array}$$

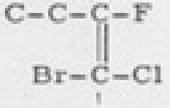
trans

C3C([=]CKB)E

D. ONE ENUMERATED GROUP ATTACHED.
   cis—enumerated group and heavier group of unenumerated pair on same side of double bond
   trans—enumerated group and heavier group of unenumerated pair on opposite sides of double bond

EXAMPLE:

(18)



$$\begin{array}{ccccccc} \overset{4}{C}&-&\overset{3}{C}&-&\overset{2}{C}&-&F\\ &&&&\|&&\\ &&Br&-&\underset{1}{C}&-&Cl\end{array}$$

cis

CKB(=)CFE

(19)

$$\begin{array}{ccccccc} \overset{4}{C}&-&\overset{3}{C}&-&\overset{2}{C}&-&F\\ &&&&\|&&\\ &&Cl&-&\underset{1}{C}&-&Br\end{array}$$

trans

CKB[=]CFE

E. NO ENUMERATED GROUP ATTACHED.
   cis—heavier group of each pair on same side of double bond
   trans—heavier group of each pair on opposite sides of double bond.

EXAMPLE:

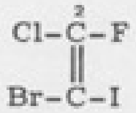
(20)

$$\begin{array}{ccccc} Cl&-&\overset{2}{C}&-&F\\ &&\|&&\\ I&-&C&-&Br\end{array}$$

trans

CBJ[=]CFK

(21)



$$\begin{array}{ccccc} Cl&-&\overset{2}{C}&-&F\\ &&\|&&\\ Br&-&C&-&I\end{array}$$

cis

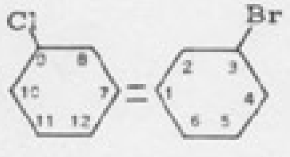
CBJ(=)CFK

8.1 DELINEATION OF CIS-TRANS CONFIGURATIONS AT ACYCLIC DOUBLE BOND CONNECTING TWO RINGS

The two ring paths attached to each of the ring atoms connected by the acyclic double bond concerned are considered to constitute a pair of enumerated paths. The cis-trans designations are defined as follows:
   cis—lower numbered ring path of each pair on same side of double bond
   trans—lower-numbered ring path of each pair on opposite sides of double bond

EXAMPLE:

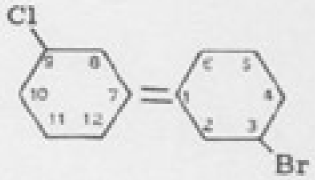
(1)



cis

6L((=)@LLLKL3)LLBL3

(2)



trans

6L([=]@LLLKL3)LLBL3

8.2 DELINEATION OF CIS-TRANS CONFIGURATIONS AT OLEFINIC RING BONDS. SYMBOLS (:) and [:]

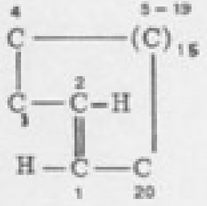
The two enumerated ring paths attached to the ring atoms connected by the olefinic ring bond in question are considered to constitute two enumerated groups attached to different atoms of the two connected by the double bond concerned.

The symbol (:) denotes cis ring double bond; the symbol [:], trans ring double bond
   cis—both enumerated groups (ring paths) on same side of double bond
   trans—both enumerated groups on opposite sides of double bond

EXAMPLE:

(1)

(2)



cis

trans

2ΔL(:)LLL9L9

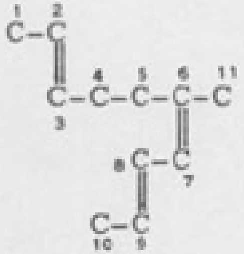
2ΔL[:]L9L9

8.3 DELINEATION OF CIS-TRANS CONFIGURATIONS IN MOLECULES CONTAINING MORE THAN ONE DOUBLE BOND

The procedure described above is applied to each double bond configuration as though it were the sole double bond in the molecule. Where the cis-trans configuration is unknown, or undefined, use the generic double bond symbol "=" to represent the double bond concerned.

EXAMPLES:

(1)

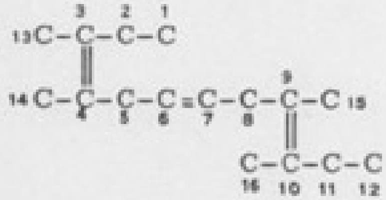


2,3 configuration - trans

6,7 configuration - trans
8, 9 configuration - trans

cipher: MC[=]CCCCM[=]CC[=]CM

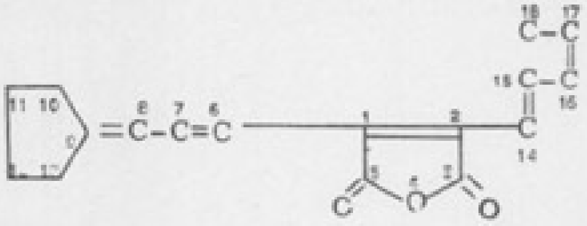
(2)



3,4 - Cis; 6,7 - generic; 9,10 - trans

ECM(=)CMCC=CCCM[=]CME

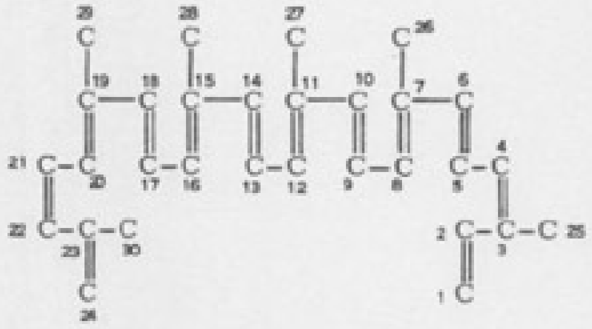
(3)



6,7-generic; 8,9-generic; 14,15-trans; 16,17-cis

5L(C=C–C=@5LL4):L(C[=]CC(=)CM)LVOLV

(4)

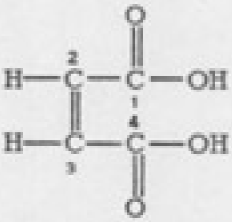


$\text{C=C}\overset{3}{\text{C}}\text{M [=] C}\overset{5}{\text{C}}\text{ [=] C}\overset{7}{\text{C}}\text{M(=)C}\overset{9}{\text{C}}\text{ = C}\overset{11}{\text{C}}\text{M(=)}\overset{12}{\text{C}}\text{C [=]}$
$\overset{14}{\text{C}}\text{CM(=)CC [=] CCM(=)CC(=)CCM=C}$

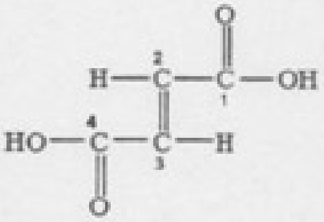
configurations:

3,4-trans; 5,6-trans; 7,8-cis
9,10-trans; 11,12-cis; 13,14-trans
15,16-cis; 17,18-trans; 19,20-cis
21,22-cis

(5)



(6)



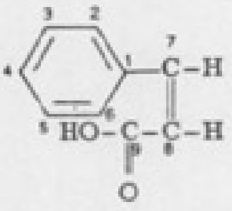
cis

trans

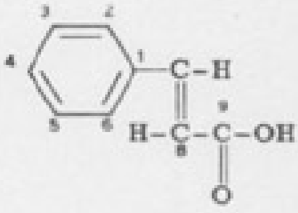
CVQC(=)CCVQ

CVQC[=]CCVQ

(7)



(8)



cis

trans

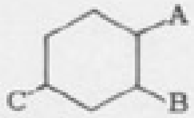
6R(C(=)CCVQ)R5

6R(C[=]CCVQ)R5

8.4 Cis-Trans ISOMERISM IN CYCLIC STRUCTURES

The type of isomerism considered here is characterized by the projection of substituent groups on the same side or on opposite sides of the plane of the ring to which such groups are attached. In the following description rings are considered as lying in the plane of the paper. Groups attached to a ring by a solid line lie above the plane of the paper; those attached by a dotted line lie below the plane of the paper.

EXAMPLE:



Groups A and B lie above the plane of the paper; group C, below.

8.41 DELINEATION OF Cis-Trans CONFIGURATION RELATED TO RING PLANES. SYMBOL "a".

First, enumerate the structural formula of the molecule and proceed to cipher same. For a given planar ring system the first ciphered

(1) isomeric skeletal substituent,
(2) isomeric functional substituent, or the
(3) isomeric hydrogen atom occupying the lowest numbered fused position in the order of decreasing priority is the reference group.

All ciphered substituents of the given ring system which lie on the same side of the plane of the system as the reference group are ciphered in the usual way. The ciphers of all substituents which lie on the opposite side of the plane from the reference group are suffixed by the lower-case letter "a" to denote the "anti" or "trans" configuration.

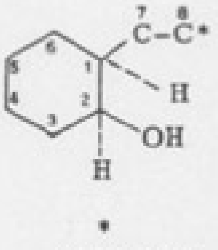
If the substituent cipher ends with a closing parenthesis the "a" symbol immediately follows said parenthesis.

In all other cases place the "a" symbol immediately after the last symbol of the substituent cipher concerned.

The cipher serves to indicate the relative positions of the substituent groups with respect to the plane of the ring. It is not necessary to cipher the stereochemical configuration of a hydrogen atom, unless it is bonded to a fused atom and is "anti" (opposite side of the plane) to the reference group, as described in the next section. The sterechemical configuration of a hydrogen atom bonded to an unfused ring atom is inferred as being always opposite to that of a ciphered group attached to the same ring atom.

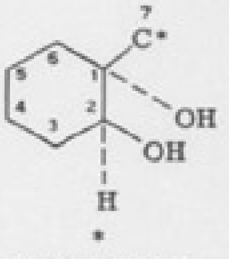
EXAMPLES (asterisks indicate reference groups):

(1)



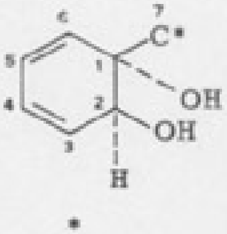
6LELQL4

(2)



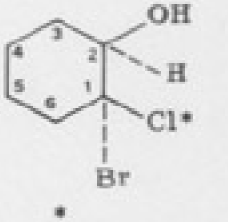
6LQaMLQL4

(3)



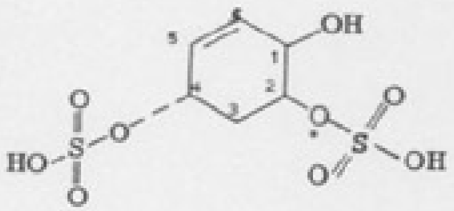
6LQaMLQL:LL:L

(4)



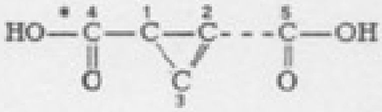
6LKBaLQL4

(5)



LQL(OSWQ)LL(OSWQ)aL:L

(6)



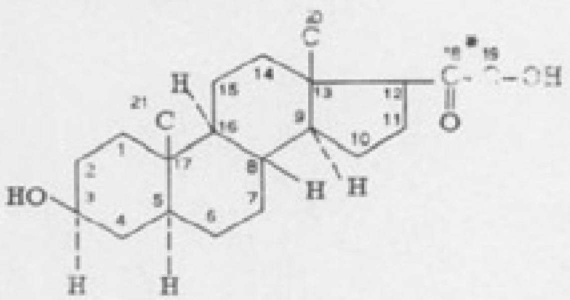
3L(CVQ)L(CVQ)a:L

8.42 STEREO-CHEMICAL HYDROGEN ATOMS.

Hydrogen atoms attached to ring carbon atoms are not ciphered unless the ring carbon to which a hydrogen atom is attached occupies a fused position, and then only if the hydrogen atom in question lies on the opposite side of the plane from the reference group, in which case the hydrogen configuration is indicated by placing after the Y symbol the lower case letter "a", which follows a ring size numeral when cited.

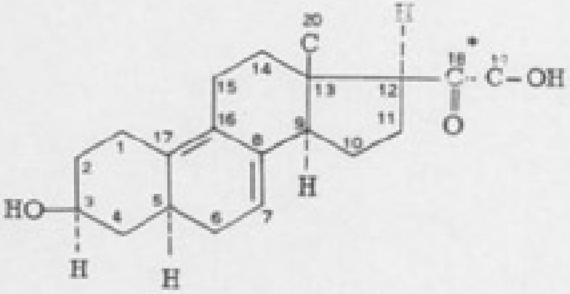
EXAMPLES:

(1)



6LLLQLYaLLYY5aLLL(CV$\dot{\text{C}}$Q)YMLLYaYM

(2)



6LLLQLYaLL:YY5aLLL(CV$\dot{\text{C}}$Q)YMLLY:Y

If the steric relations are known at only some of the positions, then the first ciphered

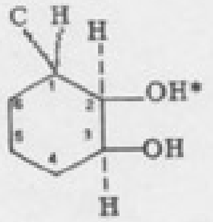
(1) isomeric skeletal substituent, or

(2) isomeric functional substituent,

in the order of decreasing priority, of which the steric relation is known becomes the reference group. The symbol "a" is placed after the ciphers of only those groups which are known to be trans-related to the reference group.

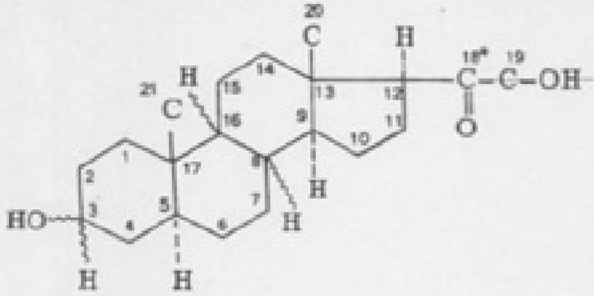
EXAMPLES (a wavering bond indicates that the cis-trans relations of the substituent attached is unknown):

(3)



6LML$\dot{\text{Q}}$LQL3

(4)



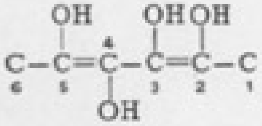
6LLLQLYaLLYY5aLLL(CV$\dot{\text{C}}$Q)YMLLYYM

8.5 ENUMERATION OF CONTENDING PATHS WHICH ARE UNSYMMETRICAL SOLELY WITH RESPECT TO Cis-Trans RELATIONS.

Enumerate the above described paths in the order in which their respective orders of ascending enumeration assign the lower number on the occasion of the first difference to a skeletal atom to which is bonded a substituent, excluding all hydrogen attached to carbon except ortho-fused, which has a "cis" relation in the enumerated path concerned.

Each substituent attached to a "cis" double bonded atom is considered "cis"; and each substituent of a "trans" double bonded atom, considered "trans". In ring paths a "cis" substituent is one which lies on the same side of the ring plane as its reference group as explained above.

(1) (1)

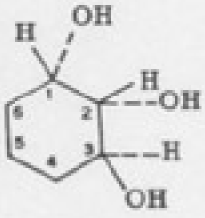


$$\underset{6}{C}-\underset{5}{\overset{OH}{C}}=\overset{4}{\underset{OH}{C}}-\underset{3}{\overset{OH}{C}}=\underset{2}{\overset{OH}{C}}-\underset{1}{C}$$

MCQ (=) CQCQ[=]CQM

In (1) atom 2 bears an OH substituent which is cis, whereas corresponding atom 5 bears a "trans" OH group. The ascending enumeration shown assigns the lower number to an atom, atom 2, which bears a cis substituent on the occasion of the first difference.

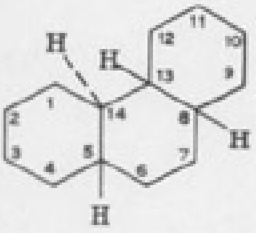
(2)



6L$\dot{\text{Q}}$LQLQaL3

In (2) the atoms which stand in final contention for selection as starting atom are atoms 1 and 3, based on feature 2a. of Section 2.61 which eliminates atoms 4, 5, and 6. The first difference concerned occurs at atom 2 whose substituent is cis with respect to the OH attached to atom 1 but trans with respect to the OH bonded to 3. The 1-2 sequence shown therefore generates the first "cis" substituent and the correct enumeration pattern.

(3)



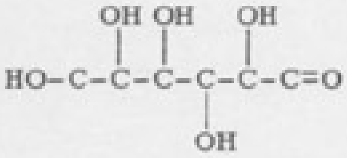
6L4YLLYL4YYa

In formula (3) the hydrogen atom bonded to position 13 is the decisive "cis" substituent.

8.6 OPTICAL ISOMERISM

Any organic molecule which contains an atom, called "asymmetric", to which four different groups are covalently bonded in a tetrahedral configuration exists in two forms with respect to the arrangement of such groups in space. The two forms, which are mirror images of each other, are called optical isomers, or "enantiomorphs", and differ only in their behavior toward light which is polarized in a single plane. One isomeric form rotates plane polarized light to the right (clockwise) and is called "dextrorotatory"; the other, to the left (counter-clockwise) and is called "levorotatory". A given molecule may have a plurality of asymmetric centers, each having its own absolute configuration and each contributing additively to the optical property of the molecule as a whole.

In order to represent the tetrahedral configuration of a given asymmetric center by an unambiguous planar projection Emil Fischer introduced (1891) a convention (See Ref. 11, p.262) using D-glyceraldehyde as a model, whereby, in its simpler form, the carbon chain is drawn as a straight line with side groups, e.g. the hydroxy groups of glucose, oriented perpendicular to the chain, as indicated below:



$$\mathrm{HO{-}C{-}\overset{OH}{\overset{|}{C}}{-}\overset{OH}{\overset{|}{C}}{-}\underset{OH}{\underset{|}{C}}{-}\overset{OH}{\overset{|}{C}}{-}C{=}O}$$

D (+) glucose

It is permissible to rotate the projection formula in the plane of the paper as long as the arrangement of the groups is not disturbed.

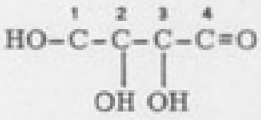
The present notation follows the Fischer convention for establishing the planar projection formulas of optical isomers but does not establish any particular molecule as a reference standard. Instead, the tetrahedral configuration at each asymmetric center is delineated by executing the following operations in the order listed:

1. Establish the planar projection formula of the molecule, according to the Fischer convention for representing the tetrahedral configuration.
2. Enumerate the projection formula and orient it, by rotation only, horizontally with the lower numbered atom which is attached to the asymmetric center concerned disposed to the left (west).
3. Beginning with the lower numbered atom described by item 2, proceed to cipher the molecule in the usual manner until the asymmetric atom is ciphered, then cipher the substituents thereof in the regular manner except that after the cipher of any such substituent - hydrogen bonded to carbon not ciphered - which is oriented upward (north) place the symbol "a."
4. As the final item of the molecular cipher place the symbol "(+)", if the molecule as a whole is specified as dextrorotatory and the symbol "(-)", if levorotatory.

When it desired to show the isomeric configurations of repeating chain units, e.g., the "$-\underset{\mathrm{OH}}{\underset{|}{\mathrm{C}}}-$" units in the eight aldohexoses in the examples below, such units are not multiplied, as would otherwise be the case for a series of three or more non-terminal chain units.

EXAMPLES:

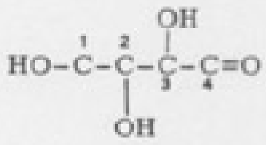
(1) Erythrose:



$$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\underset{|}{\overset{2}{C}}}{-}\underset{OH}{\underset{|}{\overset{3}{C}}}{-}\overset{4}{C}{=}O}$$

CQCQCQCV

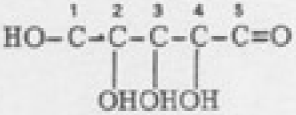
(2) Threose:



$$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\underset{|}{\overset{2}{C}}}{-}\overset{OH}{\overset{|}{\underset{3}{C}}}{-}\underset{4}{C}{=}O}$$

CQCQCQaCV

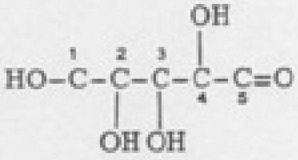
(3) **Ribose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{OH}{\overset{3}{C}}{-}\underset{OH}{\overset{4}{C}}{-}\overset{5}{C}{=}O}$

CQCQCQCQCV

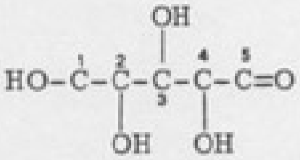
(4) **Arabinose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{OH}{\overset{3}{C}}{-}\underset{4}{\overset{OH}{C}}{-}\underset{5}{C}{=}O}$

CQCQCQCQaCV

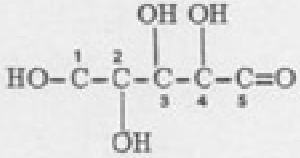
(5) **Xylose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{OH}{\overset{4}{C}}{-}\overset{5}{C}{=}O}$

CQCQCQaCQCV

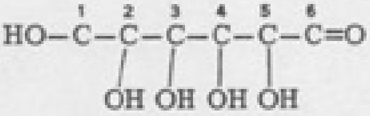
(6) **Lyxose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{4}{\overset{OH}{C}}{-}\underset{5}{C}{=}O}$

CQCQCQaCQaCV

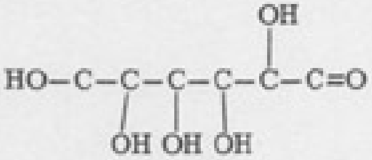
(7) **Allose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{OH}{\overset{3}{C}}{-}\underset{OH}{\overset{4}{C}}{-}\underset{OH}{\overset{5}{C}}{-}\overset{6}{C}{=}O}$

CQCQCQCQCQCV

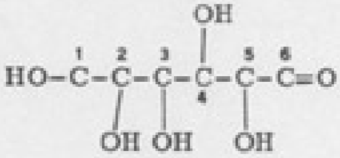
(8) **Altrose:**



$\mathrm{HO{-}C{-}\underset{OH}{C}{-}\underset{OH}{C}{-}\underset{OH}{C}{-}\overset{OH}{C}{-}C{=}O}$

CQCQCQCQCQaCV

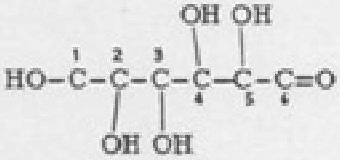
(9) **Glucose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{OH}{\overset{3}{C}}{-}\underset{4}{\overset{OH}{C}}{-}\underset{OH}{\overset{5}{C}}{-}\overset{6}{C}{=}O}$

CQCQCQCQaCQCV

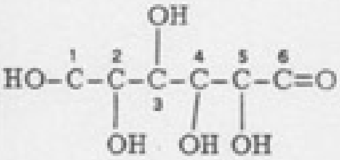
(10) **Mannose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{OH}{\overset{3}{C}}{-}\underset{4}{\overset{OH}{C}}{-}\underset{5}{\overset{OH}{C}}{-}\underset{6}{C}{=}O}$

CQCQCQCQaCQaCV

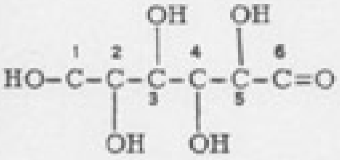
(11) **Gulose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{OH}{\overset{4}{C}}{-}\underset{OH}{\overset{5}{C}}{-}\overset{6}{C}{=}O}$

CQCQCQaCQCQCV

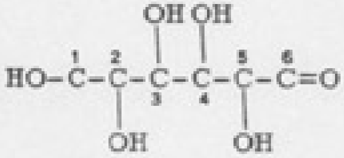
(12) **Idose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{OH}{\overset{4}{C}}{-}\underset{5}{\overset{OH}{C}}{-}\overset{6}{C}{=}O}$

CQCQCQaCQCQaCV

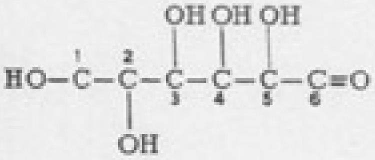
(13) **Galactose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{4}{\overset{OH}{C}}{-}\underset{OH}{\overset{5}{C}}{-}\overset{6}{C}{=}O}$

CQCQCQaCQaCQCV

(14) **Talose:**



$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{4}{\overset{OH}{C}}{-}\underset{5}{\overset{OH}{C}}{-}\underset{6}{C}{=}O}$

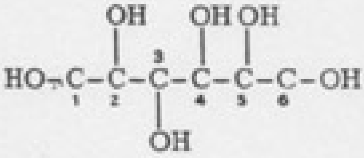
CQCQCQaCQaCQaCV

8.7 ENUMERATION OF CONTENDING PATHS WHICH ARE UNSYMMETRICAL SOLELY WITH RESPECT TO OPTICAL CONFIGURATIONS

Enumerate the above described paths in the order in which their respective orders of ascending enumeration assign the <u>lower number on the occasion of the first difference to an asymmetric skeletal atom to which is bonded an optical "a"</u> substituent when the enumerated projection formula is oriented, by rotation only, with the lower numbers disposed to the left (west) in a horizontal plane, as described by operation 2 of Sec. 8.6.

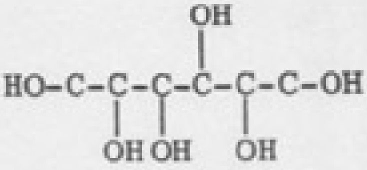
EXAMPLES:

D - Sorbitol A.



$\mathrm{HO{-}\underset{1}{C}{-}\underset{2}{\overset{OH}{C}}{-}\underset{OH}{\overset{3}{C}}{-}\underset{4}{\overset{OH}{C}}{-}\underset{5}{\overset{OH}{C}}{-}\underset{6}{C}{-}OH}$

CQCQaCQCQaCQaCQ

B. 

$$\mathrm{HO{-}C{-}\underset{OH}{C}{-}\underset{OH}{C}{-}\overset{OH}{C}{-}\underset{OH}{C}{-}C{-}OH}$$

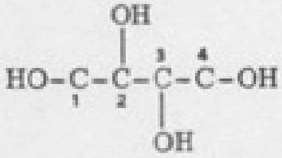
The A formula is correctly enumerated in compliance with the foregoing rule.

8.8 OPTICAL ISOMERS HAVING SYMMETRICAL HALVES

When the above described halves are <u>not mirror images</u> of each other orient the projection formulas, enumerated from either end, horizontally with the lower numbers to the left, as described above, then place the symbol "a" after the cipher of each upwardly oriented substituent of an asymmetric atom.

EXAMPLES:

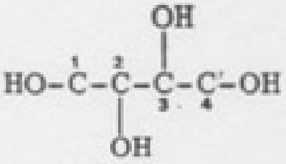
D (levo) - tartaric acid:

(1) 

$$\mathrm{HO{-}\underset{1}{C}{-}\underset{2}{\overset{OH}{C}}{-}\underset{OH}{\overset{3}{C}}{-}\overset{4}{C}{-}OH}$$

CQCQaCQCQ(-)

L (dextro) - tartaric acid:

(2) 

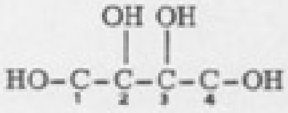
$$\mathrm{HO{-}\overset{1}{C}{-}\underset{OH}{\overset{2}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{4}{C}{-}OH}$$

CQCQCQaCQ(+)

When the above described halves are <u>mirror images</u> of each other the molecule is described as optically "meso", in which case the molecule is enumerated from either end and ciphered as though no optical configuration existed for the molecule, i.e., all "a" symbols related to optical relations are omitted.

EXAMPLE:

Meso-tartaric acid:



$$\mathrm{HO{-}\underset{1}{C}{-}\underset{2}{\overset{OH}{C}}{-}\underset{3}{\overset{OH}{C}}{-}\underset{4}{C}{-}OH}$$

CQCQCQCQ

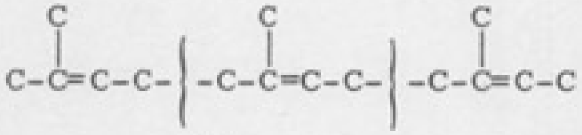
9.0 POLYMERS. SCHEMATIC REPRESENTATION

For purposes of enumeration and ciphering a polymer is represented schematically as consisting of <u>two end structures and a repetitive middle structure</u>. The <u>end structures</u> represent the residues of the monomers from which the polymer was formed and may be the same, in the case of homopolymers, or different in the case of copolymers.

The <u>repetitive middle structure</u> represents the smallest repeating unit which is directly connected to, but does not include, a skeletal atom of the lowest-numbered end structure and which unit together with the end structures account for all atoms of the polymeric molecule.

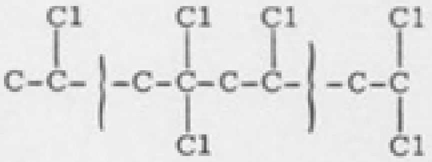
In each of the formulas below those portions which lie outside of the braces are end structures; the portion enclosed by braces is a repeating middle unit.

EXAMPLES:

(1) 

$$\mathrm{C{-}\overset{C}{C}{=}C{-}C{-}\Big\{{-}C{-}\overset{C}{C}{=}C{-}C{-}\Big\}{-}C{-}\overset{C}{C}{=}C{-}C}$$

polyisoprene

(2) 

$$\mathrm{C{-}\overset{Cl}{C}{-}\Big\{{-}C{-}\underset{Cl}{\overset{Cl}{C}}{-}C{-}\overset{Cl}{C}{-}\Big\}{-}C{-}\underset{Cl}{\overset{Cl}{C}}}$$

"SARAN"

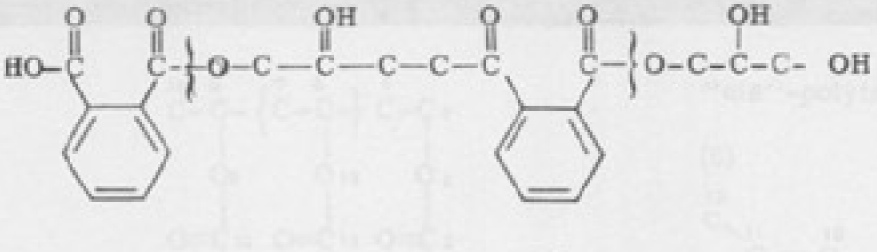
(3) $\mathrm{C{-}C{-}\{{-}C{-}C{-}\}{-}C{-}C}$

polyethylene-1, 2

$$\mathrm{C{-}C{-}\{{-}\underset{C}{C}{-}\}{-}C{-}C}$$

polyethylene-1, 1

(4)



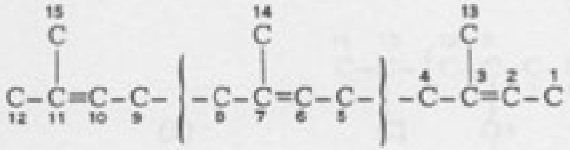
polyglyceryl-pathalate

9.1 ENUMERATION OF A POLYMER FORMULA

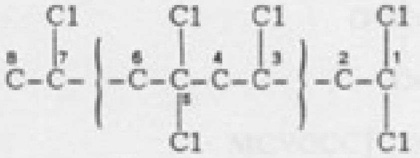
The formula of a polymer, constructed as described above, is enumerated as though it represented a monomeric molecule except that the enumeration must begin with an end structure.

EXAMPLES:

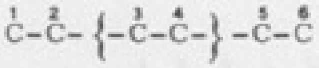
(1)



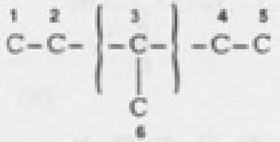
(2)



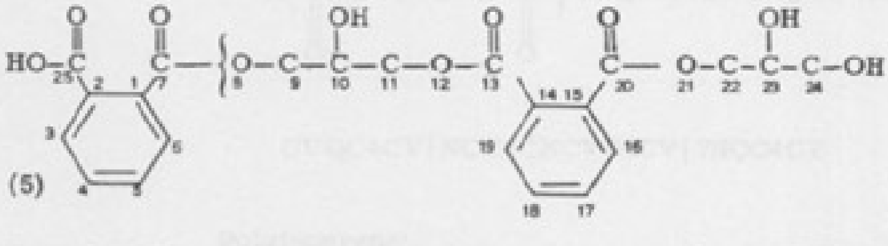
(3)



(4)



(5)



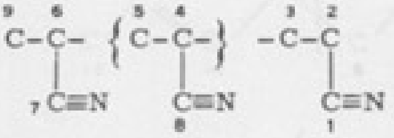
Note that the repeating unit is directly connected to a skeletal atom "7" of the lower numbered monomer residue, or phthalyl rather than the glyceryl residue (atoms 21-24).

9.2 CIPHERING OF ACYCLIC POLYMERIC MOLECULES

The schematic formula is first constructed and enumerated as described above. The resulting formula is ciphered as though it represented a monomeric molecule, except that the braces are retained in the cipher in the same relative positions as in the formula and are suffixed by a question mark "?". To indicate that the number of repeating units is known, substitute the numerical value for "?". If the number of units is less than 3 the compound is not characterized as a polymer and is ciphered in the regular way without the use of braces or the ? symbol.

"ORLON" (polyacylonitrile):

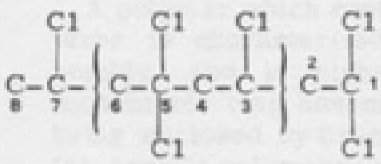
(1)



C(÷N)CC{C(C(÷N))C}?CMC(÷N)

"SARAN" (vinyl chloride - vinylidene chloride):

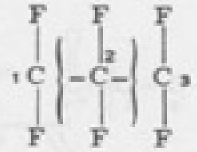
(2)



CK2C{CKCCK2C}?CKM

"TEFLON" (polytetrafluoroethylene):

(3)

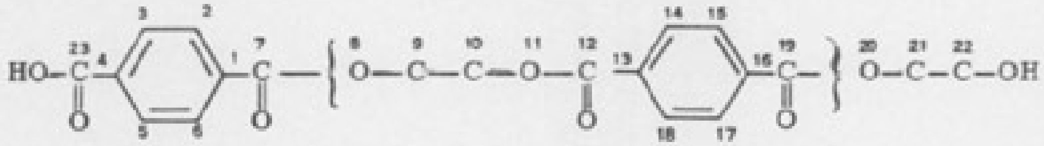


CF2{CF2}?CF2

Polyvinyl-acetate:

"DACRON":

(2)

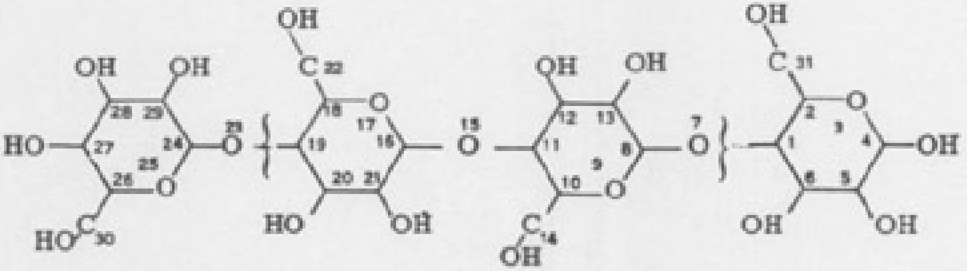


$\text{6R(CV\{OCCOCV@6RRRR(}\underset{6}{\text{C}}\text{V/OCCQ)/}\overset{17}{\text{R}}\text{R\}?)}\overset{2}{\text{R}}\overset{3}{\text{R}}\overset{4}{\text{R}}\text{R}$

(CVQ)RR

Cellulose:

(3)



$\text{6L(}\overset{7}{\text{O}}\text{@6L}\overset{9}{\text{O}}\text{L(CQ)}\overset{11}{\text{L}}\text{(O@6}\overset{16}{\text{L}}\text{OL(CQ)}\overset{19}{\text{L}}\text{(/}\overset{23}{\text{O}}\text{@}\overset{24}{\text{6}}\text{LOL(CQ)}$

LQLQLQ)/LQLQ)LQLQ}?)L(CQ)OLQLQLQ

The enumeration and ciphering procedures illustrated above are intended to be applied only to polymeric molecules whose structures are known and can be accurately represented by schematic formulas of the type described.

10.0 ORGANIC SALTS. DEFINITION

An organic salt is a carbon compound constituted by two or more ions of opposite charge. The ions may either be separate entities, as exemplified by the sodium salts of fatty acids, or composited in a single organic species wherein the charges are separated by covalently bonded atoms, as exemplified by an amino acid. In this notation the electrical charge exhibited by an organic ion is not attributed to any given atom (or atoms) thereof but rather to the ion as a whole.

10.1 INORGANIC IONS. CIPHERING ORDER

Inorganic ions are ciphered by citing first that atom of the ion which has

(1) the highest valence state, or the
(2) heaviest atomic weight

in the order of decreasing priority, followed by the elemental symbols (multiplied where necessary to show number of occurrences) of all other atoms arranged left to right in the order of their increasing weights.

All ions are enclosed by brackets. A bracket inherently present due to an element symbol serves as enclosure and is never doubled. See arsenate and metaborate, below.

EXAMPLES OF ANIONS:

Name	Anion Formula	Cipher
Hydroxide	OH	[OH]
Arsenate	AsO_4^{-3}	[AS]O4]
Sulfate	$SO_4^{=}$	[SO4]
Bisulfate	HSO_4^{-}	[SHO4]
Iodate	IO_3^{-}	[IO3]
Metaborate	BO_2^{-}	[BO]O2]
Tetraborate	$B_4O_7^{=}$	[BO]4O7]

Name	Cation	Cipher
Chlorate	$ClO_3^=$	[KO3]
Chlorplatinate	$PtCl_6^=$	[PT]K6]
Trimolybdate	$Mo_3O_{10}^-$	[MO]3O1A]
Nitrate	NO_3	[NO3]
Nitrite	NO_2	[NO2]
Perborate	BO_3	[BO]O3]
Perchromate	CrO_8	[CR]O8]
Permanganate	MnO_4	[MN]O4]
Phosphate (monobasic)	H_2PO_4	[PH2O4]
Phosphate (dibasic)	HPO_4	[PHO4]
Phosphate (tribasic)	PO_4	[PO4]
Phosphite (ortho)	HPO_3	[PHO3]
Thioantimonate	$SbS4$	[SB]S4]
Tungstate	WO_4	[WO]O4]

A metal cation which is stable in more than one valence state is suffixed by a number equal to the valence thereof.

EXAMPLES OF CATIONS:

Name	Cation	Cipher
Aluminum	Al^{+3}	[AL]
Ammonium	$NH4^+$	[NH4]
Antimonous	$S6^{+3}$	[SB]3
Antimonic	$S6^{+5}$	[SB]5
Arsenous	Ar^{+3}	[AR]3
Arsenic	Ar^{+5}	[AR]5
Calcium	Ca^{+2}	[CA]
Chromous	Cr^{+2}	[CR]2
Chromic	Cr^{+3}	[CR]3
Cuprous	Cu^{+1}	[CU]1
Cupric	Cu^{+2}	[CU]2
Hydrogen	$H+$	[H]
Magnesium	Mg^{+2}	[MG]
Manganous	Mn^{+2}	[MN]2
Manganic	Mn^{+3}	[MN]3
Molybdenum II	Mo^{+2}	[MO]2
Molybdenum III	Mo^{+3}	[MO]3
Molybdenum IV	Mo^{+4}	[MO]4
Molybdenum VI	Mo^{+6}	[MO]6
Molybdenum VIII	Mo^{+8}	[MO]8
Osmium II	Os^{+2}	[OS]2
Osmium III	Os^{+3}	[OS]3
Osmium IV	Os^{+4}	[OS]4
Osmium VIII	Os^{+8}	[OS]8
Nickelous	Ni^{+2}	[NI]3
Nickelic	Ni^{+3}	[NI]3

Ciphering inorganic ions in the manner described avoids any necessity for establishing the nature of bonding between the atoms thereof and yet represents each ion unambiguously. In addition there can be no mistaking the cipher of an inorganic ion for that of a functional substituent.

10.2 SALTS OF ORGANIC ACIDS AND INORGANIC CATIONS. CIPHERING

A salt of an organic acid wherein the cation is inorganic is ciphered by executing the following operations in the order given:

1. Cipher the inorganic ion(s) in the manner described above.
2. Cipher the organic acid anion as though in the free acid state and enclose the cipher by brackets "[ ]".
3. If the organic acid anion occurs more than once in the salt indicate the number of such occurrences by the appropriate numerical prefix before the introductory anion bracket: 3[ ]
4. Indicate the number of charges, if more than one, on the acid anion by the appropriate numerical suffix after the closing anion bracket: [ ]2
5. Arrange the ciphers produced by operations 1-4 above on a line, cation cipher to the left and anion cipher to the right, and separate the former from the latter by a semi-colon: [ ] ; [ ].
6. When a salt contains a plurality of cations and/or anions, arrange the ciphers of such ions to the left and right of the semi-colon, as described by rule 5, and the ciphers of ions of like charge in the order of their increasing weights, separated from one another by commas as indicated below:

[ ], [ ]; [ ], [ ]

In the event a salt contains a plurality of organic ions of like charge which ions have the same weight but different configurations arrange their ciphers in the order in which their respective enumeration patterns assign the lower number on the occasion of the first difference to the following features listed in their order of decreasing priority:

1. skeletal atom to which is bonded the greater number of hydrogen atoms in the saturated hydrocarbon state of the organic species concerned;
2. features listed in Sec. 2.61 in their same order of priority.

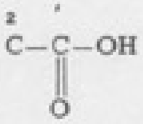
In the following examples the ciphers are developed in the order of the above operations.

SALTS OF MONO BASIC ORGANIC ACIDS

(1) SODIUM ACETATE

ration cipher: [NA]

free acid formula:



$\overset{2}{C}-\underset{\underset{O}{\|}}{\overset{1}{C}}-OH$

free acid cipher: CVQM

acid anion cipher: [CVQM]

salt cipher: [NA] ; [CVQM]

(2) ALUMINUM ACETATE

cation cipher: [AL]

anion cipher: 3 [CVQM]

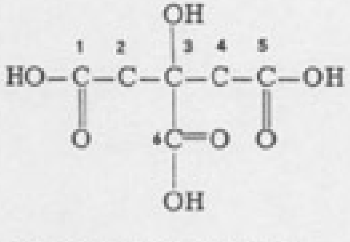
salt cipher: [AL] ; 3[CVQM]

SALTS OF POLYBASIC ORGANIC ACIDS

(3) MONOSODIUM CITRATE

cation cipher: [NA]

free acid formula:



free acid cipher: CVQCCQ(CVQ)CCVQ

anion cipher: [CVQCCQ(CVQ)CCVQ]

salt cipher: [NA] ; [CVQCCQ(CVQ)CCVQ]

(4) DISODIUM CITRATE

cation cipher: 2 [NA]

free acid cipher: same as above

anion cipher: [CVQCCQ(CVQ)CCVQ]

salt cipher: 2 [NA] ; [CVQCCQ(CVQ)CCVQ]

(5) SODIUM POTASSIUM LITHIUM CITRATE

cation cipher: [LI] , [NA] , [KA]

free acid cipher: same as above

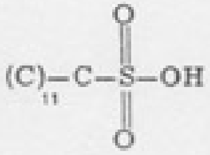
anion cipher: [CVQCCQ(CVQ)CCVQ]

salt cipher: [LI], [NA], [KA] ;
[CVQCCQ(CVQ)CCVQ]

(6) SODIUM LAURYL SULFONATE

cation cipher: [NA]

free acid formula:



$(C)_{11}-C-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-OH$

free acid cipher: C(SWQ)C9E

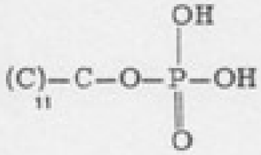
anion cipher: [C(SWQ)C9E]

salt cipher: [NA] ; [C(SWQ)C9E]

(7) LITHIUM LAURYL PHOSPHATE

cation cipher: [LI]

free acid formula:



$(C)_{11}-C-O-\overset{\overset{OH}{|}}{\underset{\underset{O}{\|}}{P}}-OH$

acid cipher: C(OPVQ2)C9E

anion cipher: [C(OPVQ2)C9E]

salt cipher: [LI] ; [C(OPVQ2)C9E]

(8) DILITHIUM LAURYL PHOSPHATE

cation cipher: 2 [LI]

acid cipher: same as above

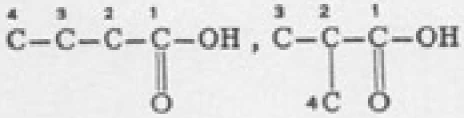
anion cipher: [C(OPVQ2)C9E] 2

salt cipher: 2 [LI]; [C(OPVQ2)C9E] 2

(9) **CALCIUM BUTYRATE ISOBUTYRATE**

cation cipher: [CA]

free acid formulas:



$$\overset{4}{C}-\overset{3}{C}-\overset{2}{C}-\underset{\underset{O}{\|}}{\overset{1}{C}}-OH\ ,\ \overset{3}{C}-\underset{\underset{{}^{4}C}{|}}{\overset{2}{C}}-\underset{\underset{O}{\|}}{\overset{1}{C}}-OH$$

anion ciphers: [CVQC3] , [CVQT]

salt cipher: [CA] ; [CVQC3] , [CVQT]

10.3 AMINE ADDITION SALTS. QUATERNARY AMMONIUM SALTS

The nitrogen atom of amine salts is ciphered as pentavalent, the fifth valence in each case being expressed as a positive charge. All four groups which are covalently bonded to the nitrogen atom, including hydrogen atoms, if any, constitute the cation state of the amine and are ciphered as such. In the event a plurality of amino groups occur in the same ionic species each amino group is ciphered in the tetracovalent state, i.e. with an additional hydrogen at each amino nitrogen in the case of an amine addition salt and with the quaternizing group cited at each such nitrogen atom in the case of a quaternary ammonium salt. The number of amino nitrogens actually involved in salt formation is indicated by the numeral which prefixes the anion species. The ions of amine salts are bracketed with the appropriate prefixes and suffixes and arranged in the manner described above for other salts.

EXAMPLES:

(1) Methyl amine hydrochloride:

Amine formula: $C\text{-}NH_2$

Anion cipher: [K]

Cation cipher: [CNH3]

Salt cipher: [CNH3];[K]

(2) Dimethyl amine hydrochloride

Amine formula:

$$C-\overset{H}{N}-C$$

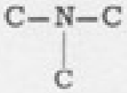
Anion cipher: [K]

Cation cipher: [NH2M2]

Salt cipher: [NH2M2];[K]

(3) Trimethyl amine hydrochloride:

Amine formula:



$$C-\underset{\underset{C}{|}}{N}-C$$

Anion cipher: [K]

Cation cipher: [NHM3]

Salt cipher: [NHM3];[K]

(4) Tetramethyl ammonium chloride:

Anion cipher: [K]

Cation cipher: [NM4]

Salt cipher: [NM4];[K]

(5) Ethylene diamine monohydrobromide:

Amine formula: $H_2N-C-C-NH_2$

Anion cipher: [B]

Cation cipher: [CNH3CNH3]

Salt cipher: [CNH3CNH3] ; [B]

(6) Ethylene diamine dihydrobromide:

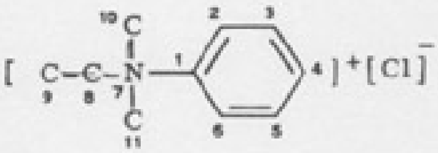
Anion cipher: 2[B]

Cation cipher: [CNH3CNH3]

Salt cipher: [CNH3CNH3];2[B]

(7) Dimethylethyl phenyl ammonium chloride:

Formula

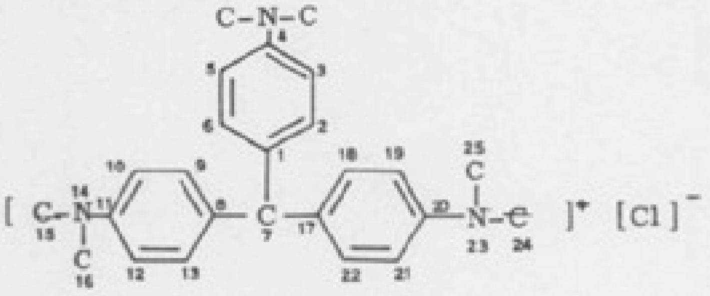


Cation cipher: [6R(NM2E)R5]

Anion cipher: [K]

Salt cipher: [6R(NM2E)R5]; [K]

(6) Crystal violet:



cation cipher: [6R(C(@6RRRR(NHM2)RR)2RRR(NHM2)RR]

anion cipher: [K]

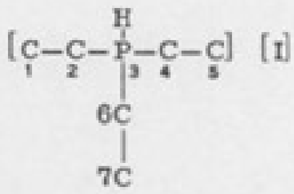
salt cipher: [6R(C(@6RRRR(NHM2)RR)2RRR(NHM2)RR];[K]

10.4 INTERMOLECULAR OXONIUM SALTS

The compounds treated here are such as are formed, as the amine salts above, by an addition reaction which increases the covalence of some atom to a higher than normal value and increases correspondingly the formal charge on the organic species containing such atom so that the species exhibits an ionic state. In all compounds of the subject type the hyper-covalent, or ''onium'', atom is ciphered in its actual state of covalency, i.e. with all multiple bonds and covalently bonded groups ciphered as if attached to carbon. In no case is the formal charge involved localized at the onium atom. Instead the charge is expressed as an attribute of the ionic species as a whole and indicated by a numerical suffix after the closing ion bracket, if the charge is greater than one.

(1) Triethyl phosphonium iodide:

Formula



$$[\mathrm{\underset{1}{C}{-}\underset{2}{C}{-}\overset{H}{\underset{3}{P}}{-}\underset{4}{C}{-}\underset{5}{C}}]\ [\mathrm{I}]$$

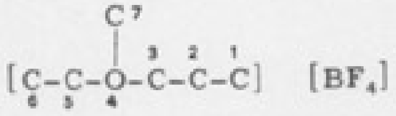
$$\mathrm{P}\,|\,\mathrm{6C}\,|\,\mathrm{7C}$$

cation cipher: [PHE3]

anion cipher: [I]

salt cipher: [PHE3];[I]

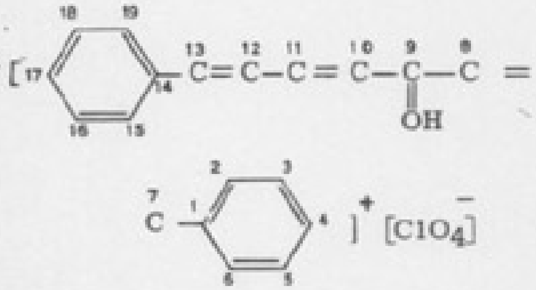
(2) Methylethylpropyloxonium borotrifluoride:

Formula 

$$[\mathrm{\underset{6}{C}{-}\underset{5}{C}{-}\overset{C^{7}}{\underset{4}{O}}{-}\overset{3}{C}{-}\overset{2}{C}{-}\overset{1}{C}}]\quad[\mathrm{BF_4}]$$

salt cipher: [CCCOME];[BO]F4]

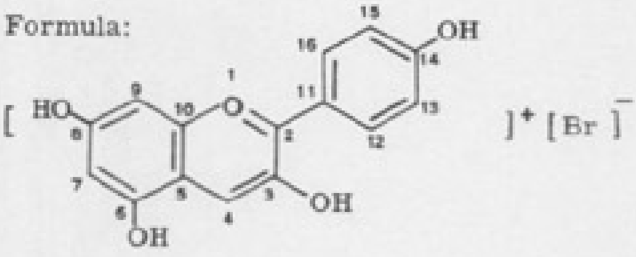
(3) Benzalcinnamalacetone perchlorate:

Formula: 

salt cipher: [6R(C=CC(=Q)C=CC=C@6RR5)R5];[KO4]

(4) Pelargonidin bromide:

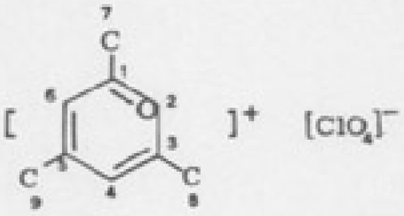
Formula:



salt cipher: [6OR(@6RRRRQRR)RQRYRQRRQRY];[B]

(5) Trimethylpyroxonium perchlorate:

Formula:



salt cipher: [6RMORMRRMR];[KO4]

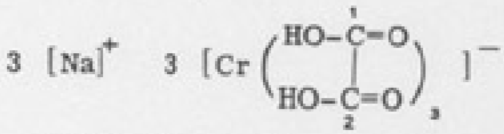
10.5 METAL CHELATES.

The coordinating metal atom is ciphered as a cation without charge. The coordinating organic entity is ciphered in the free state and represented as an anion without charge. All other ions which are not engaged in chelate linkages are ciphered with charge. The opening brackets of both the coordinating metal cation and the coordinating organic anion are prefixed by an arabic numeral to denote the number of occurrences of each, if greater than one. The closing bracket of each chelating entity is suffixed by a period "." to denote chelate character.

EXAMPLES:

(1) Sodium trioxalato chromiate:

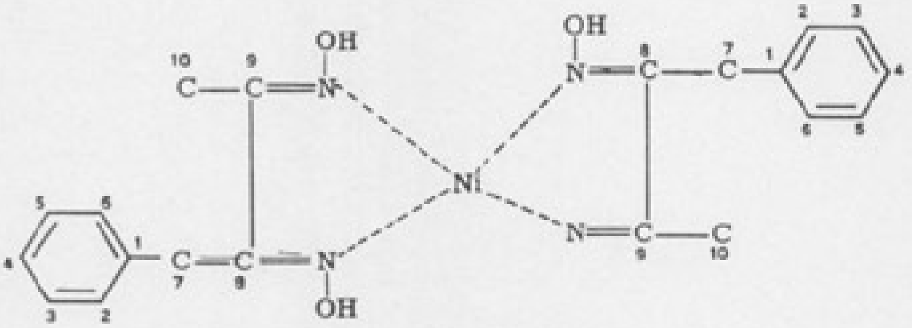
Formula:



$$3\ [\mathrm{Na}]^{+}\quad 3\ \left[\mathrm{Cr}\left(\begin{matrix}\mathrm{HO{-}\overset{1}{C}{=}O}\\ |\\ \mathrm{HO{-}\underset{2}{C}{=}O}\end{matrix}\right)_{3}\right]^{-}$$

salt cipher: 3 [NA], [CR].; 3 [CVQCVQ].

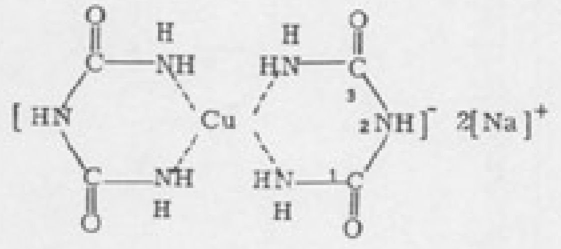
(2) Nickel benzylmethyl glyoxime:



salt cipher: [Ni].; 2 [6R(CC(=NQ)C(=NQ)M)R5].

(3) Biuret copper:

Formula:

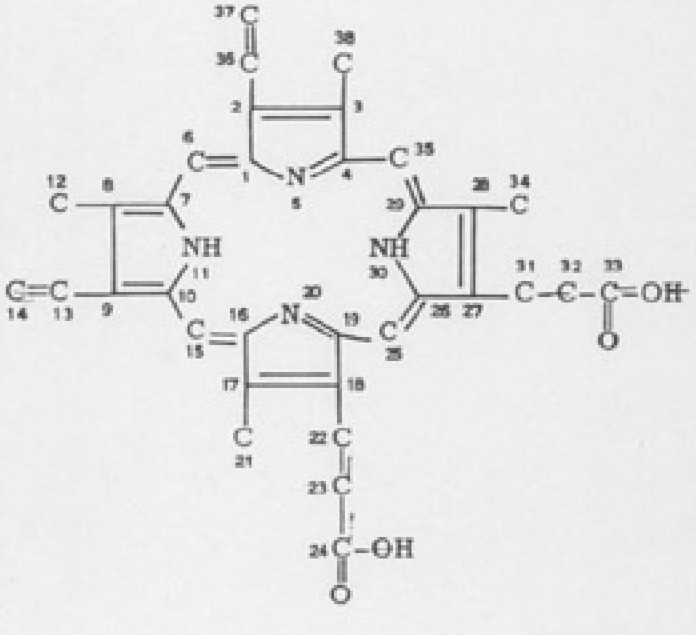


salt cipher: 2 [NA], [CU].; 2 [N(HCVZ].

See 2.8-3.

(4) Haemin:

Formula:



cipher: [FE].; [5$\overset{1}{\text{L}}$(=C@5$\overset{7}{\text{L}}$:LML(C=C):$\overset{10}{\text{L}}$(C=@5
$\overset{16}{\text{L}}$LM:$\overset{18}{\text{L}}$(CCCVQ)L(C=@5LL(CCCVQ):LML
(=$\overset{35}{\text{C}}$@)nH):n)nH$\overset{2}{\text{L}}$(C=C):LML( ):n].

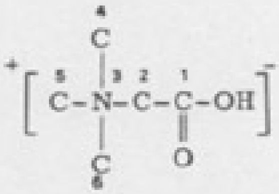
The ciphering of metal chelates in the manner described deliberately avoids characterizing the nature of chelate bonding because of the controversial nature of such bonding and the variety of ways in which such bonding may be represented.

10.6 INTRAMOLECULAR SALTS.

Internal salts, wherein both salt forming groups are part of the same molecule, and such groups consequently, cannot be separated by an electric field, are ciphered in the "free state" and the cipher thereof enclosed by brackets.

EXAMPLES:

(1) Betaine:

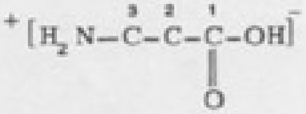


cipher: [CVQCNM3] *

*The 5th valence of nitrogen is expressed by the brackets.

β-amino-propionic acid:

Formula:

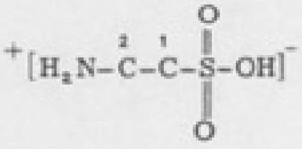


$^{+}[\mathrm{H_2N{-}\overset{3}{C}{-}\overset{2}{C}{-}\underset{\underset{O}{\|}}{\overset{1}{C}}{-}OH}]^{-}$

cipher: [CVQCCZ]

(2) Taurine:

Formula:

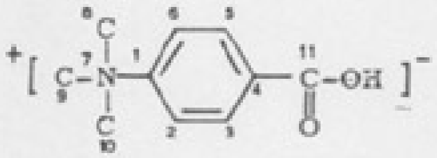


$^{+}[\mathrm{H_2N{-}\overset{2}{C}{-}\overset{1}{C}{-}\underset{\underset{O}{\|}}{\overset{\overset{O}{\|}}{S}}{-}OH}]^{-}$

cipher: [C(SWQ)CZ]

(3) Aminobenzoic acid betaine:

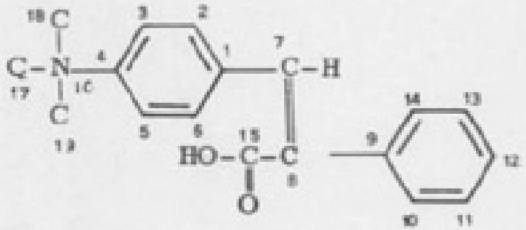
Formula:



cipher: [6R(NM3)RRR(CVQ)RR]

(4) p-Amino-α-phenyl-cis-trans-cinnamic acid-trimethyl betaine:

Formula:



trans-cipher: [6R(C(CVQ)($\overset{*}{=}$)C@6RRRR(NM3)RR)
R5]

cis cipher: same as trans except double bond expressed as [=]

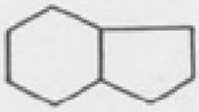
---

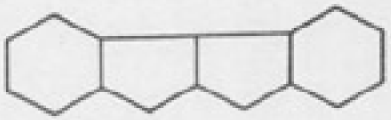
*See Sec. 8.20B.

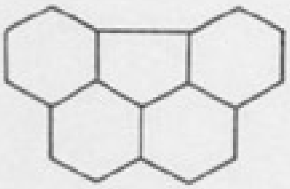
11.0 DECIPHERING

The reconstruction of a structural formula from its cipher is essentially a process of reconstituting the vertical dimension by which ring structure and chain branching is expressed. It is a forte of line formula notation that the bonding relationships among the atoms and configurations of a given compound are retained directly in the cipher thereof. Consequently, in deciphering the present notation there is no need for recourse to seniority rules or to reestablish an enumeration pattern, as is required by "locant" notation wherein the molecule is represented by disjointed fragments.

In reconstituting fused ring systems it is perhaps more straightforward to construct each ring in its entirety as a geometric polygon from the ring sizes which are expressed by the cipher and then filling in the atoms, rather than by generating each ring atom by atom. A template is a very convenient device for the rapid construction of rings, particularly a template which includes regular polygons of 3, 4, and 6 sides in a variety of sizes. Such devices are usually available at stores which merchandise stationary and/or art materials. To make 5 and 6 membered rings fit together properly construct each 5 membered ring with the same sized hexagon used to construct 6 membered rings of the same formula, by establishing (by template) four sequential sides of the hexagon then closing the ring by a longer side of the necessary length. In joining other rings to a given 5 membered ring by ortho fusion it is perhaps more convenient to leave the described longer side of the 5 membered ring free whenever possible and to maximize the use of the shorter sides which form a right angle with the longer side as shown below:





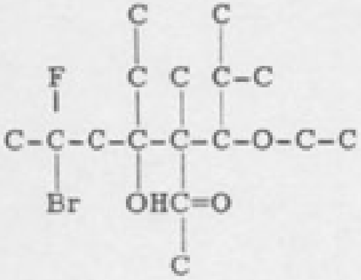


In some cases, of course, it may be necessary to resort to free hand reconstruction of fused rings when the angles of contiguous polygons become incompatible with the template design.

In constructing substituents of a chain atom orient each substituent path perpendicular, wherever possible, to the related parent path.

EXAMPLE:

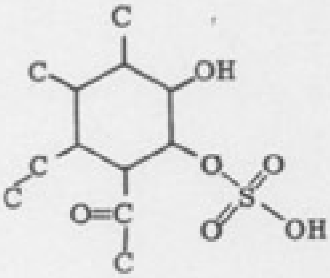
(1)



In attaching substituents to rings orient each substituent in as steep an angle as possible with respect to the sides of the polygon which include the ring atom involved.

EXAMPLE:

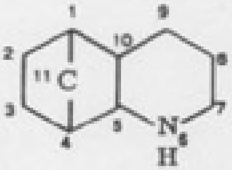
(2)



To reconstruct the bridges of a bridged ring system note the identifying number which terminates each bridge (introduced by asterisk) and connect the terminal bond of the bridge to that atom of the parent ring system whose symbol in the cipher is suffixed by the same identifying number.

EXAMPLE:

(3)

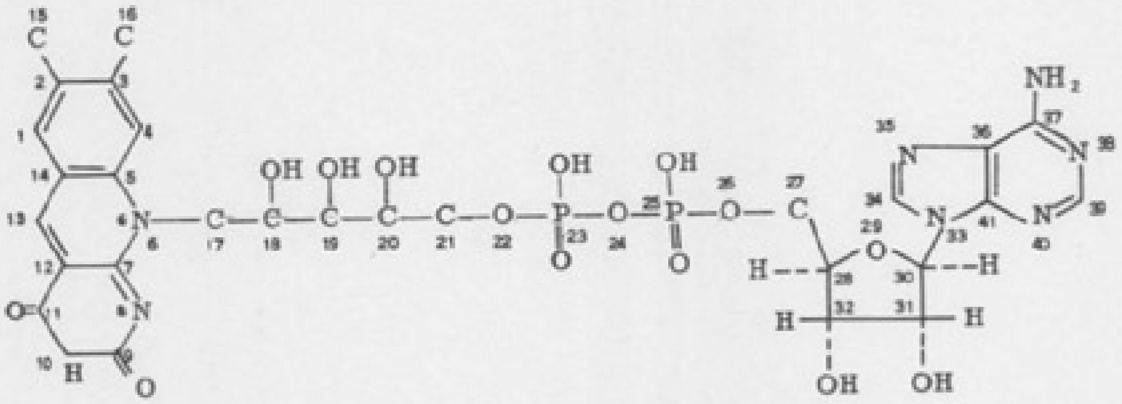


6L*L(1)LLL(1)YnHLLLY

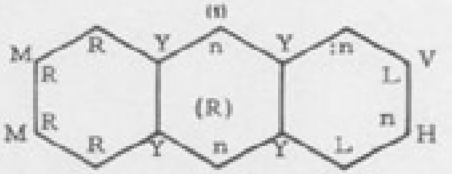
Any cipher which contains the symbol "@" represents a ring assembly. A count of the number of @ symbols plus one indicates the number of component ring systems in a random assembly. In a circular ring assembly the number of @ symbols is equal to the number of component ring systems. If one of the @ symbols is followed immediately by a closing parenthesis "@)" the component ring systems are joined in a closed path so as to form a circular ring assembly. If an inspection of the cipher indicates, by the number of @ symbols and/or by the number of total symbols, that the structural formula will spread over a relatively large area it may be simpler to construct each component ring system and the connecting linkages independently, identifying the points of connection by appropriate numerals as illustrated below by the formula and cipher of Riboflavin adenine dinucleotide:

Riboflavin adenine dinucleotide:

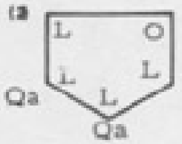
4

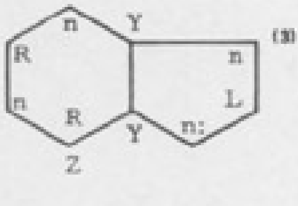


```
          12 3 4 6 17       22        27
cipher:  6RRMRMRYn(C {CQ} 3COPVQOPVQOC@
            33 35         41 31 32   7 8  10
         5LOL(@5nL:nYRZnRnY5)LQaLQa)Y:nLVnH
                        12 14
                       LVY:nY
```



(1)CCQCQCQCOPVQOPVQOC(2)





Each ring system is reconstructed by ignoring the substituents thereof, that is by skipping over all of the cipher symbols which are included within the opening and closing parentheses which define the boundaries of the substituent concerned or otherwise indicate substituency, e.g., M. In the mechanical method of Isaacs and Walker (see Preface) this operation of ignoring a given substituent is performed by adding to a count-box, pre-set to zero, the quantity "one" for each successive opening parenthesis "(", beginning with the one which introduces the substituent in question, and subtracting from the same count-box the same quantity for each successive closing parenthesis ")". The return of the count-box to the zero state signals the end of the substituent and that the next cipher symbol encountered resumes the parent path, provided that the next symbol itself does not indicate a substituent.

APPENDIXES

A. Ciphers of Miscellaneous Compounds Selected From Fieser and Fieser.[11]

B. Ciphers of 100 Compounds From IUPAC Test List.[8]

C. Ciphers of Test Compounds[8] Submitted to IUPAC by G.K.D.

APPENDIX A: Ciphers of representative organic compounds whose structural formulas appear in Fieser and Fieser at the page locations indicated by the parenthesized number to the left of each cipher. Indentation of a row of symbols indicates a continuation of the row immediately preceding.

(29) C7
C4T
C3CME
C3CM3
ECMT
CT2
CE2M2
CE3
TCM3

(31) C9M
C9C9E
 C9C9C9C3
C9{C9}4C5

(47) 3L3
4L4
5L5
 6L6

(53) C=C
C=CM
 C=CE
 MC=CM
C=CM2
C=CC3
C=CME
C=CT
C=CC4
C=CC5
C=CC6

(79) C(CM2E)2

(80) C=CMCCM3
CKC3CQ
EC=C(C3)CMCE2
C=CC=CC=C
 CQC=C

(81) C3C(CQ)E
5LMLML3
6LELQLLLQL
6R(@5LL:LLL)R5
6RMRMR4
6RMRRMR3
6RMRRRMRR

(85) C÷C
C÷CM
 C÷CE
 MC÷CM
C÷CT
 C÷CC9C7

(99) 6RMR3YRRMRMnY
6RMRRMnYR(CME)R3Y

(112) CQCE
 CQT
MCQE
CM3Q
MQ
EQ
CQC=C

(113) [NA] ; [CVQC7C=CCCQC4E]

(124) CKCQCQ
CQCQCQ
CVQCQCQ

(131) C(ONW)C(ONW)C(ONW)

(132) C(CQ)4
C(C(ONW))4

(133) MOM
MOE
 EOE
ECOCE
TOT
MOCCE
EOCCE
 ECCOCCE
ECCCOCCCE
TCCOCCT
EC3COCC3E
CKOCK
CKCKOE
CKCOCCK

MOCCOM
C=COC=C
C=CCOCC=C
5OLLLL
6R(O@6RR5)R5
6R(OM)R5
(134) MCQOOCQM
(137) [MOM] ; [K]
(138) [EOE] ; [BO] F3]
(140) CBCCBC4CVOE
C(SH)CC(SH)C4CVQ
5L(C4CVQ)SSLL
(146) MK
EB
TI
CKCE
CBT
MCBE
MCBM2
(154) CK2
CK3
CF4
CF2K2
CKCK
CK2M
CK3CK3
CK=CK
(163) CVQ
CVQM
CVQT
CVQCF
CK3CVQ
CVQCQ
CVQCQM
CVQC(SH)
CVQCC(≡N)
CVQCV
6R(CCVQ)R5
(174) CVOM
CVOE
MOCVM
MCVOE
MCVOCT
(176) C(=NH)Z(NHNW)
C(=NH)(NHNW)NHM
C(=NH)(NHNW)N(NV)M
6R(SWN(NV)M)RRRMRR
(180) CVFM
CVKCK
CVKT
6R(CVK)R5
(186) MCVOCVM
5OLVLLLV
6R4Y5LVOLVY
(188) CV=C
CVQCCCVZ
MOCVCCCVQ
(192) CV
CVM
CK3CV
CVCV
CVE
5L(CV)OL:LL:
MCVM
MCVE
MCVC3
MCVCM3
MCVCVM
6LVLL3L
(193) 6LTLQLLMLL
6LTLVLLMLL
(204) TC(O [MG] B)T
(207) AL [(OT)3]
(209) MCVCCQM2
MCVC=CM2
MCM=CCVC=CM2
(211) C(=NQ)M
MC(=NQ)M
(212) 6R(NHN=C@6RR5)R5
CVZ(NHZ)
CVZNHN=CM
(213) 6n*LnΔL(1)L(2)Ln(1)Ln(2)L
(217) EOCVCCVM
EOCVC=CQM
(218) EOCVCCVOE
EOCVCCVM
MCVCCVM
(225) MZ
MNHM
NM3
EZ
ENHE
NE3
CZC9E
CZCZ
CZC4CZ
CQCZ
CQCN(CCQ)2
6RZR5
(227) [MNH3] ; [K]
[ENH3] ; [K]
[ENH2E] ; [K]
[NHE3] ; [K]
[6R(NH3)R5] ; [K]
(228) [NM4] ; [I]
[NM4] ; [OH]
(231) 6R(NHCVM)R5
C(=NQ)C6
5L(=NQ)L4
(234) 6R4Y5LVnHLVY
(240) [NVM3]
(243) CVZCCCVZ
CVQCZ
5nBLVLLLV
CVZ2
(245) 6nHLVnHLVY5 {:} nHLVnHY
6nRQnRQY5nHLVnHY
6nHLVnHLVLQ2LV

6nRQnRQRRQ

5nHLVnHLVLV

(247) 6nMLVnMLVY5 {:} nML:nY

6nMLVnMLVY5 {:} nHL:nY

6nMLVnHLVY5 {:} nML:nY

6nRnRY5n:LnHY

(262) CQCQCV(+)

(263) CVQCQaCQ(-)

CVQCQaM(-)

CVQCQCCVQ(-)

CVQCQCQaCVQ(-)

(264) CVQCQCQCQaCQCV(+)

(265) 6R(CBaCBCVQ)R5(+ -)

6R(CBCBaCVQ)R5(+ -)

6R(CBaCBaCVQ)R5(+ -)

6R(CBCBCVQ)R5(+ -)

(266) CVQCKaCQaCVQ(+-)

CVQCKCQCVQ(+ -)

CVQCKaCQCVQ(+-)

CVQCKCQaCVQ(+-)

(268) CVQCQaCQCVQ(-)

CVQCQCQaCVQ(-)

CVQCQCQCVQ(-+)

(291) 3L(CVQ)L(CVQ)aL

3L(CVQ)LCVQ)L

(293) 2 [NA] ; [6R(CVNH@6RRR(SWQ)R(C=C@6RR(SWQ)RR(NHCV@6RR(OM)R4)RR)RR)R(OM)R4]

(296) 3L(C7CVQ):L(C8)L

(299) 6L4YL4Y

6L4YL4Ya

(301) CVQC7C(=)CC8

(311) 6L*O(1)LLL(1)Y5MLVOLVYM

(320) CVC5C=CC7CVC(CVM)CVOE

(324) 5L(CQCQ)OLVLQLQ

(348) 6LTLQaLLMaLL

6L*L(1)LM2L(1)LKMLL

6L*LM2(1)MLKLL(1)LL

(352) 6R(NHN=CC({CQ}3CQ)=NNH@6RR5)R5

(355) CQCQCQCQaCQCV

CQCQCQCQaCQaCV

CQCQCQCQaCVCQ

CQCQCQaCQaCQCV

(363) 6L(OM)OL(CQ)LQLQLQ

5L(OM)OL(CQCQ)LQLQ

(365) 8L(OM)OL(CQ)LVO [SR] OLV

(366) 6LQa(CQ)OLLQLQLQa

5LQa(CQ)OL(CQ)aLQLQa

(379) 6L(O@6RRRRQRR)OL(CQ)LQaLQLQa

(380) 6L(CO@6LL(OM)aL(OM)L(OM)aL(COM)O)L(OM)aL(OM)L(OM)aL(OM)O

(386) 6L({O@6LOL(CQ)L(O@6LOL(CQ)L/(O@6LOL(CQ)LQaLQLQa)a/LQLQa)a LQLQa}?)L(CQ)aOLQLQLQa

(391) 5L(CQCQ)OLVLQ=LQ

(392) 6OLM2OLY5aOY5(CQ)OLM2OY5Ya

(422) 6R(O@6RRRIRQRIR)RIRR(CCZCVQ)RRI

(424) 6R(CCZaCVQ)R5

CVQCZC(SH)

CSCCCZaCVQ

CVQCZCQ

(437) 6R(O@6RRRR(OM)RR)RIRR(CV)RRI

5SC(=S)nHLVL

(444) 6R(COCVNHC(CVQ)CCCVNHC(CVNHCVQ)CSC@6RR5)R5

(449) 6R(C@2△LLVnHL(CME)LVnHL(CCVZ)LVnHL(CCCVZ)LVnHL(CV@5nL(CVNHC(CT)CVNHCCVZ)L3)LSSLLZCVnH)RRRQRR

(465) 6RRMRMRYn(C {CQ} 3COPVQ2)Y:nLVnHLVY:nY

(467) [6R(C@5nLM:L(CCOPVQOPVQ2)SL:)RZnRMNR] ; [K]

6RZnRnY5n(@5LOL(COPVQOPVQOCCM2CQCVNHCCCVNHCC(SH))L(OPVQ2)aLQa)L:nY

(490) [C9C8CVNHC(COPVQOCCNM3)CQC=CC9C4]

(505) 6nHL(CNH@6RRRR(CVNHC(CVQ)CCCVQ)Ln(CV)YnRZnRQY

(577) 6RMR(NW)R(N(NW)M)R(NW)RR(NW)

(583) 6RMR(CVM)RMR(NW)R(CM3)R(NW)

(770) 6R(C VQ)RQRRMYLYRQRMRRQYLVY

(784) 6LLLQaLYLLQaYY5LLL(CMCCCVQ)YMLQLYYM

(798) 5L(CVOE):LML(CVOE):LMnH

(799) 6L*O(1)L(CVOM):L(CVOM)L(1)L:L

(806) 6R(@5L:LQL(=C(CVM)@6RR5)OLV)R5

(811) 6R(OM)RRR(OM)YRMRRQnY

6R(OM)RRR(OM)YRMRRnY

6R(OM)R(OM)RR(NW)YnRRRY

(813) [6nMRRR(C(÷N))YR4Y] ; [M(OSWQ)]

(814) 6nnRRYR4Y

6RnnRYR4Y

6nRnRYR4Y

6nRRnYR4Y

(815) 6OL:LL:LL

6OL:LLL:L

6OLVL:LL:L

6OL:LLVL:L

[6ORR3R] ; [K]

6OL:LLLL

(819) [6R(?CQCQCQCQaCQCV)RRQRYOR(@6RRRQRQRR)R(?CQCQCQCQaCQCV)RY] ; [?] (red)

6R(?CQCQCQCQaCQCV)RRQRYOL(=@6LL:LQLVL:L)L(?CQCQCQCQaCQCV):LY (violet)

[?] ; [6R(?CQCQCQCQaCQCV)RRQRYOR(@6RRRQRQRR)R(?CQCQCQCQaCQCV)RY] (blue)

(821) [6R(OM)RMRQRYOR(@6RR5)RRY] ; [K]

6L(OM):LMLVL:YOL(@6RR5):LL:Y

(827) 6L* L7LVO(1)nMLML(1)LL

6L3Ln(Y8)LL*L(1)YL3Ln(Y8)LL(1)Y

(834) 6LQaL:LYy5*nM(1)L(1)LYy5RRRQY5OY (bridge is stereo reference group)

6LQaL:LYy5*nM(1)L(1)LYy5RRR(OM)
Y5OY
6L(OM):LL:Yy5*nM(1)L(1)LYRRR(OM)
Y5OY
(839) 7L*nM(1)LLL(1)LLQL(bridge is ref. group)
7L*nM(1)LLL(1)LLQaL
7L*nM(1)LLQaLL(1)Y3OY7
5nML*L(1)LQY5OL(1)LY5 (scopoline)
(840) 6L*LL(1)nML(1)LLQL
6L*LL(1)nML(1)LLVL
6L*LL(1)nML(1)LLQaL
(841) 6LL(CVQ)LnMYLY5y:LnHYR3YY:
(842) 6LL(CVNH@5LMLVn(Y)L(C@6RR5)LVn
(Y5)LLLYY5QO)LnMYLY5y:LnHYR3
YY:
6L(CVOM)LQLLYLn(Y)LLY5 {:} YR4Y5
nHYYLYa (ref. group is CVOM)
(843) 6L(CVOM)L(OM)aL(OCV@6RRR(OM)R
(OM)R(OM)R)LYaLn(Y)LLY5 {:} YRRR
(OM)RY5nHYYLYa
(844) 7L*L(1):LLOYyLLVn(Y5)yYR4Y5Y6,5LL
n(1)YLY7
6R(CVOCCNE2)RRRZRR
(936) 6LLM:LLY3LM2Y
5L(=C)LLY3TLY5
6L*L(1)LM2L(1)LM:LL
6L*LM2(1)MLLL(1)LL
(937) CQC[=] CMCCC CM2
CQC[=] CMC3CM=C
(939) 6LM2L(C=CCVM)LM:LLLM
6LM2L(C=CCVM):LMLLLM
6LM2L(C=CCVM)L(=C)LLLM
(941) 6L*LM2(1)MaLKaLL(1)LL (bridge is ref
group)
6L*L(1)LM2L(=C)L(1)LL
6L*LM2(1)LVLL(1)LL
(943) 6L*LM2(1)MaLQLL(1)LL
(946) 7RMRRRTRY5RMRRY7
7RMR3RMY5RRTRY7
7LMLLL(CQM2)LY5 {:} LMLLY7
(947) 9L(=C)LLL(:)LMLLY4LM2LYa
9L(=C)LLL [:] LMLLY4LM2LYa
11LM2LLLMLL3LML3
7L*(1)LM2L3YMaL(=C)L(1)LLY7
7LM2L*L(1)LM:LLY5(1)LMLLY7
9L*L(1)QaL3L(1)MaLLY4LM2LYa
8LLL*L(1)MaL3Y5L:LLM2Y8
(948) 6LL:LTL:YLLYLM(CVQ)aL3YMYa
6LLLT:LY:LLYLM(CVQ)aL3YMYa
6LLL(CM=C)L:YLLYLM(CVQ)aL3YMYa
6LLL(=CM2)L:YLLYLM(CVQ)aL3YMYa

(951) 6LLLQLM2YLLY {:} Y5MaLLL(CMCCC
=CM2)YMLLY {:} YM
6LLLQLM2YLL:YY5MaLLL(CMCCC
=CM2)YMLL:YYM
6LLM2LLYMLLYMaYMLLYLM2LQLL
YMYaLL:YY
6LMLMLLYMLLYMaYMLLYLM2LQLL
YMYaLL:YY

6LLQLM2YLLYMYMaLLY5MLLL(CM
=C)YaYLLYaYM
(954) 6LM2L(C [=] CCM [=] CC [=] CCM
CCQ):LML3
6LM2L(C[=] CCM[=] CC[=] CCM(=)C
CQ):LML3

(962) 6LLLQLYaLLYY5aLLL(CMC3T)YMLL
YaYM
6LLLQLYLLYY5aLLL(CMC3T)YMLL
YaYM
(964) 6LLLQLY:LL:YY5LLL(CMC[=] CCET)
YMLLYYM
6LLLQLY:LLYY5LLL(CMC [=] CCET)
YMLLYYM
(989) 6L*OLV(1)LL(1)(CCM=C)aLQaYLL:YL
X5OLLO-LLYMY
(991) 6LLLQLYLLYY5QLLL(@5L:LLVOL)Y
MLLYaYM
(993) 6LLLQLYLLYY5QLLL(@6L:LOLVL:L)
YMLLQYYM
(994) 6OLLMLLX5OY5LYYLLYaLLQLLYM
YLLY5MY5LM
(995) 6LLLQLY:LLYY5LY5n(Y)LLMLLY5LM
Y5YMLLYYM
(1001) 6RMnRZRMRn
(1003) 6RRMRMRYn(CCQaCQaCQaCQ)Y:nLVnH
LVY:nY
(1004) 6RMR(OM)R(CVQ)R(CVQ)Rn
(1007) 6nR(CNH@6RRRR(CVNHC(CVQ)CCCVQ)
RR)RnYnRZnRQY
(1009) [C(+N)([CO])]. [6RRMRMRY5n(@5LLQ
L(OPVQOCMCNHCVCC@5LML(CCVZ)
L(@5LML(CCVZ)ML(CCCVZ)L(CM@5
LL(CCVZ)ML(CCCVZ)L(C@5LLM2L
(CCCVZ)L(CM@)nH)nH)nH)nHL( ))L
(CQ)aO)LnHY] .
(1015) 6RMRMRQRMYLLL(C3CMC3CMC3T)
MOY
(1018) 6R(OCVM)R(CC=CMC 5CC=CM2)RMR
(OCVM)YR4Y
(1022) 5 [NA] ; [6R(N=N@6RR(SWQ)RR(@6RRRR
(N=N@6RRZR(SWQ)RYRR(SWQ)RRY)
RR)RR)RZR(SWQ)RYRR(SWQ)RRY] 5
(1026) 6R(CQ@6Ln*LL(1)LL(C=C)L(1)L)RRnY

RRR(OM)RY
(1033) 5L(CVQ)LM2SY4L(NHCVC@6RRRRQRR
LVn(Y5)

(1034) 6L(O@5LL(O@6LL(NHM)LQaLQL(CQ)aO)
LQ(CV)aLMO)L(NHC(=NH)Z)aLQL(NHC
(=NH)Z)aLQLQa

(1035) 6L(NM2)LQ:L(CVZ)LVYQLQ:YLVYRQR
3YLQMYLY
6L(NM2)LQ:L(CVZ)LVYQLQ:YLVYRQ
RRRKYLQMYLY
6L(NM2)LQ:L(CVZ)LVYQLQ:YLVYRQR3
YLQMYLQY

(1036) 6R(CQC(CQ)NHCVCK2)RRR(NW)RR

APPENDIX B: Ciphers of 100 special compounds (Reference 9, pp. 305-53) Taken from the IUPAC Test List.

The compounds, whose ciphers follow, represent essentially the full range of ordinary complexity exhibited by organic molecules as viewed in the frame of the classical structural formula. The number, followed by a period, which appears to the left of each cipher identifies the cipher with the correspondingly enumerated compound name which appears in the list of names which follows the last cipher. In amine salts involving aromatic rings no shift in "double bonds" due to salt formation has been delineated. Indentation indicates continuation of same cipher.

1. 6LLLQLY:LLYY5LLL(CMC3T)YMLLYYM
2. 6LLLQLY:LLYY5LLL(CMC=CCET)YMLL
   YYM

3. 6LM2L(C=CCM=CC=CCM=CC=CC=CMC=
   CC=CMC=C@6LLM2LLL:LM):LML3

4. 6LM2L(C=CCM=CC=CCM=CC=CC=CMC=
   CC=CMC=C@6LLM2L3LM:):LML3

5. MC(C=CC= CMC=CC=CMCCC=CM2)= C
   {C=CC=CM} 3CCC=CM2

6. MOCVC= { CCM=CC= } 4CCV Q (Formula appears erroneous; ciphered as given)

7. 5L(C4CVQ)SLY5nHLVnHY5

8. 5L(CQCCQCQCVQ)L(CME)LL(CME)L:

9. 5L(CQCCVCCVQ)L(CME)LL(CME)L:

10. 6LM2L(C=CCM=CC=CCM=CC=CC=CMC=
    CC=CMC=C@6LLM2LLQLLM:):LMLLQL

11. 6nMLVnMLVY5 {:} nML:nY

12. 6nMLVnHLVY5 {:} nML:nY

13. 6NHLVnHLVY5 {:} nHL:nY (Keto form)

14. 6nHLVnHLVY5 {:} nHLVnHY (Keto form)

15. 6nHLVnHLVL:L (Keto form)

16. 6nHL(=S)nHLVL:L (Keto form)

17. 6LMnHL(= S)nHLVL: (Keto form)

18. 6L(C3)nHL(=S)nHLVL: (Keto form)

19. 6nRnRZY5n:LnHY (one form)

20. 6nR(CNH@6RRRR(CVNHC(CVQ)CCCVQ)
    RR)RnYnRZnRQY

21. 6RR(OCVNHM)RRY5nMY5nMLLY5MY

22. 6L*LL(1)nML(1)LL(OCVC(CQ)@6RR5)L

23. 6L(CVOM)LQLLYLn(Y)LLY5 {:} YR4Y5n
    HYYLY

24. 6L*LL(1)nML(1)L(CVOM)L(OCV@6RR5)L

25. 6R(C@6RRR(OM)R(OM)RR)nRRYRR(OM)R
    (OM)RY

26. 6R(CQ@6Ln*LL(1)LL(C=C)L(1)L)RRnYRRR
    (OM)RY

27. 7L*L(1):LLOYyLLVn(Y5)yYR4Y5Y6,5LLn
    (1)YLY7

28. 7L*L(1):LLOYyLLVn(Y5)yYRR(OM)R(OM)
    RY5Y6,5LLn(1)YLY7

29. 6LMLVL:LYMLLY5LMLVOYY:

30. 5L(C@5LLELVOL)nML:nL:

31. 6R4YLVYyRRYrYYyRRYyLVYR4YYRRYY
    RRYY

32. 6R4YLVYRZRKYnHYY {:} LVYR4YLVYLZ
    LKYnHYYLVY

33. 6RRRnYRRYYyRRYryYyRRYyYRRYnRRR
    YYLVYRRYYRRYLVYY

34. 6R4YLVYyrRRYrynYyyYR4YLVYRRYnYY

35. 6R(NH@6RRRYLVYRRR(NH@6RRRR(OM)
    YLVYR4YLVY)RYLVYR)RRR(OM)YLVY
    R4YLVY

36. 6R3R(NH@6RRRYLVYR4YLVYR)YLVYyR
    3Y:LLVnMY {:} Y

37. 6L4Y5nHL(=@5LnHYL4Y5LV)LVY

38. 6R4Y5Yy:L(@6RR5)LVn(Y5)yYR4Y5Y:L
    (@6RR5)LVn(Y5)Y

39. 6R4YLVYRY5OL(@6RRRYLVYR4YLVYR)
    :nYRYLVY

40. 6R4YLVYRRY5YrY5YRRYLVYR4YLVYY
    5nHYYLVYrY5nHYYLVYR4YLVYRRY5
    YY5YRRYLVYR4YLVYY5nHYYLVYY5
    nHYYLVY

41. 6R(NEC@6RRRR(SWQ)RR)RRR(N=N@6RRRR(NW)RR)RR

42. [NA]:[6R4Y5SL(@6RRR(SWQ)R(NHN=N@6RRRR(NW)RR)RR):nY]

43. [NA] ; [6RR(SWQ)R(N=N@6RRMR4)RQYRRY5nHYR4Y5YY]

44. 4 [NA]; [6RR(@5LSYRRMRRY5n:)RRY5n:L(@6RRR(SWQ)R(N=N@6RRZR(SWQ)R(N=N@6RRR(SWQ)R3)R(SWQ)R)RR)SY] 4

45. 3 [NA] ; [6R(N=N@5LL(CVQ):nn(@6RRRR(SWQ)RR)LQ:)RRR(SWQ)RR] 3

46. [NA] : [6R(N=N@5LLM:nn(@6RRRR(SWQ)RR)LQ:)R5]

47. 3 [NA] ; [6RR(NHCVNH@6RRMR(NHCVNH@6RRRYRQR(N=N@6RRMR4)R(SWQ)RYR)RR(SWQ)R)RRYRQR(N=N@6RRMR4)R(SWQ)RY] 3

48. 3 [NA] ; [6LL(NHCVNH@6LLML(NHCVNH@6LLLY {:} LQL(N=N@6LLLYLLL:LYL:)L(SWQ):LYL):LL(SWQ)L)LLY {:} LQL(N=N@6LLLY {:} LLL:LYL)L(SWQ):LLY] 3

49. 6R(N=N@6RRR(N=N@6RR5)RZRRZ)RRR(N=N@6RRRR(CNE2)RR)YR4Y

50. 2[NA]; [6RQR(N=N@6RRRR(N=N@6RRZRRZRR)RR)RSWQRYRR(SWQ)R(N=N@6RRRR(N=N@6RRZRRZRR)RR)RZY]

51. [6RR(NM2)RRYrnYRRR(NM2)RYSY];[K]

52. [6R(C@6RR5)@6RRRR(NHM2)RR)RRR(NHM2)RR];[K]

53. [6R(C(@6RRRR(NHE2)RR)2RRR(NHE2)RR];[K]

54. [6RR(NHM2)RRYL(@6RR5)YRRR(NHM2)RYOY;[K]

55. [6R4YL:LY:LYYR4YL:Ln(Y)HL(@6RR5)n(Y)HY];[K]

56. 6RR(NH@6RRRYrnYRRR(NH@6RRYrnYRRR(NH@6RRRZR3)RYnYR)RYnYR)RRYrnYRRR(NH@6RR5)RYnY

57. 6L(@6RR5)ELVnHLVnHLV

58. 6L(@6LL5)ELVnHLVnHLV

59. 6L(CC=C)2LVnHLVnHLV

60. 6R(CVNE2)RnRRR

61. 6L:L(@6LLVOYR4YL:)LVOYR4Y

62. 6R4Y5L(@6RRRR(OCVM)RR)2LVnHY

63. 6R(CCZM)R5

64. 6R(CQCNHM)RRQRQRR

65. [NA],[6R(NH3)nHRnHY5nH(@5LOL(COPVQOPVQOC@5LOL(@6nHRR(CVZ)RRR)LQLQ)LQLQ):LnH2Y5];[K]

66. 6LLLVL:YLLYY5LLL(CVCQ)YMLLQYYM

67. 6LLLQLYLLYY5LLLVYMLLYYM

68. 6LLLVL:YLLYY5LLL(CVM)YMLLYYM

69. 6LLLQLYLLYY5LLLQYMLLYYM

70. 6LLLVL:YLLYY5LLLQYMLLYYM

71. 6RMR3YRRRTRY

72. 6RMRRRTYRRMRRY

73. CQC=CMCCC=CMCCC=CM2

74. CVC=CMCCC=CMCCC=CM2

75. 6LM2L(C=CCVM):LML3

76. 6L(CMC=CC=CM2)LLLMLL

77. 7L(CM=C)LL:LMLY4LM2LY7

78. CQC={CMC3}3T

79. 5L(CVQ)LM2SY4L(NHCVC@6RR5)LVn(Y5)

80. 6RRMRMRYnMY:nLVnHLVY:nY

82. 5nHL:LQYR({@6RRQY5OYRQR/(@6RRQY5OYRQRY5LQ:LnHYY5YY5LQ:LnHY)/Y5LQ:LnHYY5YY5LQ:LnHY}?)RQY5OYRQRY5nHL:LQYY5YY5

83. 6L3Ln(Y)YL3Ln(Y)YL3Ln(Y)Y

84. 14LTOLTnHLTnHLTnHLTnHLTnHLTnH

85. 6L(O@5LL(O@6LL(NHM)LQLQL(CQ)O)LQ(CV)LMO)L(NHC(=NH)Z)LQL(NHC(=NH)ZLQLQ

86. 6L(O@6LOL(CQ)LLQL)L(CQ)OLQLQLQ

87. 6L(O@6LOL(CQ)LQLQLQ)L(CQ)OLQLQLQ

88. 5L(C@5L:LML(CCCVQ):L(C=@5LL(CCCVQ):LML(C@5L:LMLE:LQnH):n)nH):LELM:LQnH

89. 5L:L(C=@5LL(CCVQ):L(CCCVQ)L(C=@5LL(CCVQ):L(CCCVQ)L(=C@5LL(CCVQ):L(CCCVQ)L(=C@)n:)nH):n):L(CCCVQ)L(CCVQ):L( )nH

90. 5L(N=@5Ln:L(NH@5LnHL(NH@5L:nL(N@5)L:L)L:L)L:L)nHL( ):LL:

91. 6R4YRRYY5*Y5RnRY(1)yL:LYR3YL(1)YY

92. 5nrnnYrYnYrYr5nnnYYr5nnnYYRYYR5nnnY

93. [6R(@5n:nOLQ:L)R5]

94. [6R(C@5n:nOLQ:L)R5]

95. [6n(CCVQ)RR(CVQ)RRR]

96. 6R(CDM2)R5

97. 6R(CC@6RRRR(C(@6RR5)2)RR)RRR(C(@6RR5)2)RR

98. 6RR(SVNHCCVNHC(CVQ)CSSCC(CVQ)NHCVCNHSV@6RRRYR4YR)RRYR4YR

99. 6R(NHCVNHC{C(OCVNH@6RR5)} 4COCVNH@6RR5)R5

100. 6R4YR(C(@6RR5)(OE)C@6RR5)(OE)@6RYR4YR(C(@6RR5)(OE)C(@6RR5)(OE)@)YR4Y)YR4YR( )Y

1 Cholesterol. (5-Steren-3-ol,17-(1,5-dimethylhexyl)-10,13-dimethyl-)

2 Stigmasterol. (5-Steren-3-ol,17-(4-ethyl-1,5-dimethyl-2-hexenyl)-)

3 ∝ -Carotene. (1,3,5,7,9,11,13,15,17-Octadecanonaene,3,7,12,16-tetramethyl-1-(2,6,6-trimethyl-1-cyclohexenyl)-18-(2,6,6-trimethyl-2-cyclohenyl)-)

4 β -carotene. (1,3,5,7,9,11,13,15,17-Octadecanonaene,3,7,12,16-tetramethyl-1,18-bis(2,6,6-trimethyl-1-cyclohexenyl)-)

5 Lycopene. (2,6,8,10,12,14,16,18,20,22,24,26,30-Dotriacontatridecane, 2,6,10,14,19,23,27,31-octamethyl-)

6 Bixin. (2,4,6,8,10,12,14,16,18-Eicosanonaenedioic acid,4,8,12,16-tetramethyl-,1-methyl ester)

7 Biotin. (Thieno[3,4]imidazole-4-valeric acid, hexahydro-2-oxo-,cis-)

8 Auxin a. (1-Cyclopentene-1-valeric acid, 3,5,di-sec-butyl-α,β,δ-trihydroxy-)

9 Auxin b. (1-Cyclopentene-1-valeric acid, 3,5-di-sec-butyl-δ-hydroxy-β-oxo-)

10 Zeaxanthin. (3-Cyclohexen-1-ol,4,4 -(3,7,12,16-tetramethyl-1,3,5,7,9,11,13,15,17-octadecanonaenylene)bis[3,5,5-trimethyl-)

11 Caffeine. (Xanthine,1,3,7-trimethyl-)

12 Theobromine. (Xanthine,3,7-dimethyl-)

13 Xanthine. (2,6(1H,3H)-Purinedione)

14 Uric acid. (2,6,8(1H,3H,9H)-Purinetrione)

15 Uracil. (2,4(1H,3H)-Pyrimidinedione)

16 Thiouracil. (Uracil,2-thio-)

17 Methylthiouracil. (Uracil,6-methyl-2-thio-)

18 n-Propylthiouracil. (Uracil,6-propyl-2-thio-)

19 Adenine. (Purine,6-amino-)

20 Folic acid. (Glutamic acid,N-pteroyl-)

21 Physostigmine. (Pyrrolo[2,3-b]indol-5-ol,1,2,3,3a,8,8a-hexahydro-1,3a,8-trimethyl-, O,methylcarbamate)

22 Atropine. (8-Azabicyclo[3.2.1]octan-3-ol, 8-methyl-,O- -hydroxy- -phenylpropionate)

23 Yohimbine. (Benz[g]indolo[2,3-a]quinolizine-1-carboxylic acid,1,2,3,4,4a,-5,7,8,13,13b,14,14a-dodecahydro-2-hydroxy-, methyl ester)

24 Cocaine. (8-Azabicyclo[3.2.1]octaine-2-carboxylic acid,3-hydroxy-8-methyl-,methyl ester O-benzoate)

25 Papaverine. (Isoquinoline,6,7-dimethoxy-1-veratryl-)

26 Quinine. (2-Quinuclidinemethanol,α-(6-methoxy-4-quinolyl)-5-vinyl-)

27 Strychnine. (4,6-Methano-6H,14H-indolo [3,2,1-ij]oxepo[2,3,4-de] pyrrolo[2,3-h] quinolin-14-one,2,4a,5,5a,7,8,15,15a,15b,15c-decahydro-)

28 Brucine. (Strychnine,10,11-dimethoxy)

29 Santonin. (2-Naphthaleneacetic acid,1,2,3,4,4a,7-hexahydro-1-hydroxy-α, 4a,8-trimethyl-7-oxo-, γ -lactone)

30 Pilocarpine. (5-Imidazolebutyric acid,α -ethyl- β -(hydroxymethyl) -1-methyl-,lactone)

31 Violanthrone. (5,10-Violanthrenedione. Dinaphtha[1,2,3-cd,3 ,2 , 1 -lm]-perylene-5,10-dione)

32 Indanthrene,8,17-diamino-7,16-dichloro-. (Indanthrene is 6,15 dihydroanthra-zine-5,9,14,18-tetrone)

33 Cyananthrone. (1,14-Diazodiphenanthro[1,2,3-cd,3 ,2 ,1 -lm]perylene-5,10-dione)

34 Flavanthrone. (5,13-Diazopyranthrene-8,16-dione)

35 Anthraquinone,2,7-bis(4-methoxy-1-anthraquinonylamino)-

36 7H-Dibenzo[de,h]quinoline-2(1H),7-dione,8-(2-anthraquiononylamino)-1-methyl-

37 (Indigo) Indigotin. (2,2 -Bipseudoindoxyl)

38 Ciba Lake Red B. (6H-Indolo[3, 2, 1-de] [1,5] naphthyridine-2(3H),6-dione,1,3,5-triphenyl-)

39 Caledon Brilliant Red 3B. (Anthr[2,3] oxazole-5,10-dione,2-(2-anthraquinonyl)-)

40 Caledon Khaki 2G. (Anthra[1,2-b,4,3-b ,5,6-b'', 8,7-b'']tetrakis(naphth 2,3-g indole)-5,7,9,14,19,24,26,28,33,38-decone,6,8,25,27-tetrahydro-)

41 Azo Cardinal G. (αp-Toluenesulfonic acid, -[N-ethyl-p-(p-nitrophenylazo)-anilino]-)

42 (Nitrophenine.) Benzenesulfonic acid,5-(2-benzothiazolyl)-2-(p-phenyldiazoamino)-, sodium salt

43 Fast Bordeaux BR. (7H-Benzo [c carbazole-2-sulfonic acid, 4-hydroxy-3-o-tolylazo-, sodium salt)

44 Cotton Orange R. (m-Benzenedisulfonic acid,4-amino-5-[4-[6-(6-methyl-2-benzothiazolyl)-2- Benzothiazolyl]-2-sulfophenylazo]-2-(m-suflophenylazo)-,tetrasoidum salt)

45 Tartrazine O. (3-Pyrazolecarboxylic acid, 5-hydroxy-1-p-sulfonphenyl-4-p-sulfophenylazo-,trisodium salt)

46 Pyrazolone Yellow J. (Benzenesulfonic acid,p-(5-hydroxy-3-methyl-4-phenylazo-1-pyrazolyl)-sodium salt)

47 Azidine Fast Scarlet GGS. (1-Napththol-3-sulfonic acid,6,6'-[3,3'-(5-sulfo-2-m-tolylene) diureylene]bis [2-p-tolylzao-,trisodium salt)

48 Azidine Fast Scarlet 7BS. (1-Napththol-3-sulfonic acid, 6,6'-[3,3'-(5-sulfo-2-m-tolylene)diureylene [bis[2-(2-naphthylzao)-,trisodium salt)

82 Melanin (one form) (proposed formula) (Furo[2,3-g,4,5-e′]diindole-3,5,7,11-tetrol,polymer)

83 (Tripiperideine) 1H-Tripyrido[1,2-a,1′,2′-c,1″,2″-e]-s-triazine, tetra-decahydro-

84 (Oxyheptaisobutylidenamine) 1-Oxa-3,5,7,9,11,13-hexazacyclotetradecane,2,4,6,8,10,12,14-heptaisopropyl

85 Streptomycin. (Streptidine-4-streptobiosaminide)

86 Maltose. (D-Glucose,4-(α-D-glucosido)-)

87 Lactose. (D-Glucose,4-(β-D-glaactosido)-)

88 Urobilin. (one form) (3-Pyrrolepropionic acid,2-[3-(2-carboxyethyl)-5-(4-ethyl-5-hydroxy-3-methyl-2-pyrrylmethyl)-4-methyl-2-pyrrol-eninylidenemethyl]-5-(3-ethyl-5-hydroxy-4-methyl-2-pyrrylmethyl)-4-methyl-)

89 Uroporphyrin (one form) (4,9,14,19-Porphinetetrapropionic acid,5,10,15,20-tetrakis(carboxymethyl)-)

90 Porphyrazine. (2,7,12,17,21,22,23,24-Octazapentacyclo[16.2.1.13,6.18,11.113,16]tetradeca-1,3(24),4,6,8,10,12,14,16(22),17,19-hendecaene.)

91 6,12b[3′,4′]endo-Pyrrolobenz[j]aceanthrylene

92 Tetratriazolo [a,c,h,j]acridine

93 (Phenylsydnone) Sydonone,N-phenyl-*.(1,2,3-Oxadiaz-3-olium hydroxide,5-hydroxy-3-phenyl-,inner salt

94 (Benzylsydnone) Sydnone,N-benzyl-*. (1,2,3-Oxadiaz-3-olium hydroxide, 3-benzyl-5-hydroxy-,inner salt

95 (Nicotinic acid betaine) 3-carboxy-1-(carboxymethyl) pyridinium betaine

96 (1-Methyl,1-deutero ethyl benzene) Cumene-α-d

97 Triphenylmethyl,p,p″ -ethylene bis-

98 Cystine, N, N′ bis[N-(2-napththylsulfonyl) glycyl]-, ℓ -

99 Glucamine,N-(phenylcarbamyl)-,pentacarbanilate

100 (Dimolecular dioxydibenzalanthracene tetraethyl ether) 5,16,8,13-Dibenzenodibenzo[a,g] cyclododecin,6,7,14,15-tetraethoxy-6,7,14,15-tetra-hydro-6,7,14,15-tetraphenyl-.

APPENDIX C: Ciphers of Test Compounds submitted to IUPAC by GKD[3] (Formulas appear in reference 8 pp. 421-31.) Indentation indicates continuation of same cipher.

1. 6R(N=PK=NP(=N@6RR5)=NP(=N@6RR5)=NP(=
   NH)= N@6RR5)R3
2. 6R(N=NNHC(=NH)NHC(+N))RRRKRR
3. 6RRRQRMY7LVOYR(CQ)RQY5LOLVYY7OY
4. [CQ+[FE](C+O)(CO)=CQ](structure ciphered as
   given)
5. 5L(CVOM)L(CVOM)O[FE](O[FE]QOC(CVOM)C
   (CVOM)O[FE]QO@5[FE]OL(CVOM)L(CVOM)
   O)O
6. [FE.;[K],[5L(C=@5LLM:L(C=C)L(C=@5LLM:L
   (CCCVQ)L(=C@5LL(CCCVQ):LML(=C@)n:
   n:)nH):n)L(C=C)LM:L( )n:
7. 6PV*OPVQO(1)OP(1)VOPV(OM)O
8. E(OK2[CR]VQ)
9. 6R(N([RU](NHZ)2K)NH[RU](NHZ)2K)R5
10. 6R(SWNHSMNHSW@6RR5)RRRMRR]
11. 6R(NVONV)R5
12. 6L(ON(OCV)@6RR5)L:LLVL:L
13. [6R(NHN=N(@6RRR(NW)R3)1@6nRR3R)RRRR
    (NW)RR]
14. [6R(@5nnHOLVL:)R5]
15. 6L*(1)LL(OE)LYLL(1)OLVm(Y)
16. 6R(SSWSSWS@6RR5)R5
17. 6R(SWS3SW@6RR5)R5
18. 6R(SWS(=S)2SW@6RR5)R5
19. 6R(OC(=S)SSC(=S)O@6L:LL:LLL)R5
20. MO[SI]M2O[PB]O[SI]M3
21. [GE]([SE]E)3[SE][GE]([SE]E)3
22. 6R(@6RR(C@6RR5)R4)R(@6RR5)R4

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