A Method of Coding Chemicals for Correlation and Classification (1950)

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A METHOD OF CODING CHEMICALS

FOR

CORRELATION AND CLASSIFICATION

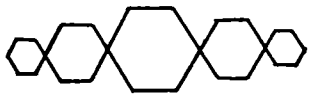

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TABLE OF CONTENTS

INTRODUCTION

In the fall of 1944, the Insect Control Committee of the Office of Scientific Research and Development (OSRD) was appointed, under the chairmanship of Dr. M.C. Winternitz (Yale University), to coordinate the work on insect and rodent control which was being carried out under OSRD sponsorship. An intensive search was conducted for new effective insecticides, insect repellents and rodenticides to protect our troops in many parts of the world from insect-borne diseases. Thousands of compounds were tested (screened) during the course of this program with the practical results of the discovery of the effectiveness of DDT in controlling malaria-bearing mosquitoes, of benzyl benzoate as a miticide, of dimethyl phthalate, butyl 3,4-dihydro-2,2-dimethyl-4-oxo-2H-pyran-6-carboxylate (Indalone) and 2-ethyl-1,3-hexanediol (Rutgers 612) as insect repellents, and of sodium fluoroacetate (1080) and 1-(1-naphthyl)-2-thiourea (ANTU) as rodenticides. Fundamental studies were also carried out on the mechanism of action of these compounds. During this time a considerable amount of information was assembled by the Committee on the effect of the structure of chemicals upon their insecticidal, rodenticidal and insect repellent action. A large amount of similar chemical-biological information was accumulated during the same period by the Board for the Coordination of Malarial Studies of the Committee on Medical Research (CMR) and the National Research Council (NRC), by the CMR and NRC Chemotherapy Center for Tropical Diseases, by the Tropical Deterioration Center of the National Defense Research Committee (NDRC) and NRC, by the Chemical Warfare Service, by Division 5, CMR and by Division 9, NDRC.

To facilitate the correlation of such data, Dr. Winternitz suggested the development of chemical and biological codes which would permit the transfer of data onto punched cards which could then be sorted on available machines. Dr. C. Chester Stock, Secretary of the Committee, investigated various chemical classification systems to determine their adaptability to a code for correlating chemical structure with biological activity. It was soon discovered that Dr. D.E.H. Frear and his associates at The Pennsylvania State College had, in 1942, devised a system for classifying chemical compounds and had used the system to classify several thousand compounds which had been tested for their insecticidal and fungicidal activity and to correlate chemical structure with these biological actions.[1] This system subsequently formed the basis from which the National Research Council Code was developed.*

Because of the war it was not possible to pursue the study of the application and modification of this coding system until the fall of 1945. At that time a group designated as the Chemical Codification Committee was formed to develop a chemical code for use with machine methods. The Committee consisted of Dr. C. Chester Stock (National Research Council), chairman, Mr. Colin Churchill (Johns Hopkins University), Dr. N.L. Drake (University of Maryland), Dr. D.E.H. Frear (The Pennsylvania State College), Drs. S.A. Hall and H.L. Haller (U.S. Department of Agriculture), Mr. John A. Morgan, Assistant to the Committee (National Research Council), Dr. A.M. Patterson (Antioch College), Dr C.A. Rouiller (Chemical Corps), Dr. E.J. Seiferle (General Aniline and Film Corporation) and Dr. E.L. Wardell (Chemical Corps). The Committee worked in close cooperation with interested groups in the Army, Navy, U.S. Public Health Service, Patent Office, Library of Congress and other government agencies as well as with interested individuals in industry and in various private and public institutions.

On July 1, 1946, the National Research Council Chemical-Biological Coordination Center was established, under the directorship of Dr. W.R. Kirner, to succeed the Insect Control Committee. The scope of the new organization was greatly broadened. Its main objectives are:

(1) To assemble and organize information which relates the effect of the structure of chemicals upon their biological activity.

(2) To sponsor the preliminary testing of chemicals on a variety of animals and plants to determine the biological effects of the compounds.

* Later, in 1947, an ingenious method of classification of organic compounds[2] was developed by Dr. G. Malcolm Dyson. This system precisely describes compounds but for effective sorting requires a special machine, which is at present not available. It has, therefore, not been possible to determine whether this system is readily applicable to correlation studies. Several other systems have also been applied to punched cards.[3]

(3) To prepare reviews of the literature on (a) the effect of chemical structure upon various biological actions; (b) test methods used in the study of such actions, etc.

(4) To sponsor symposia concerned with chemical structure-biological action problems and correlation of such data.

The following subcommittees were appointed to assist in the broad program: Biochemistry, Chemotherapy, Entomology, Malignancy, Mammalogy, Medicine, Microbiology, Organic Chemistry, Pharmacology-Physiology, Physical Chemistry, Plant Sciences, Sanitary Engineering and Veterinary Medicine. Each subcommittee chairman is a member of the Advisory Committee of which Dr. M.C. Winternitz is chairman.

Following the creation of the Chemical-Biological Coordination Center, the Chemical Coding group was constituted as the Chemical Codification Panel of the Organic Chemistry Subcommittee. The membership of this panel is identical with that previously mentioned except that Mr. Karl Heumann replaced Mr. Morgan as the NRC representative and Mr. Heumann was later replaced by Dr. Harriet A. Geer. Miss Estaleta Dale, Research Assistant to the Center, has also assisted the Panel in developing the Code during the last two years. Since it was decided to develop an inorganic chemistry section in the code, an Inorganic Chemistry Panel was appointed which was constituted as follows: Dr. John C. Bailar, Jr. (University of Illinois), chairman, Dr. L.F. Audrieth (University of Illinois), Dr. D.E.H. Frear (The Pennsylvania State College), Mr. Karl F. Heumann, Assistant to the Panel (National Research Council), Dr. C.L. Rollinson (University of Maryland), Miss Janet D. Scott (Interscience Encyclopedia), Dr. E.J. Seiferle (General Aniline and Film Corporation), Dr. C. Chester Stock (Sloan-Kettering Institute for Cancer Research), Dr Roland Ward (University of Connecticut) and Mr. W.H. Woodstock (Victor Chemical Works).

The Frear classification system and code were originally developed for use with handsorted punched cards. Because of the large number of compounds which the Chemical-Biological Coordination Center expects to handle, it was necessary to develop a code which would be used on machine-sorted cards of the IBM or Remington Rand type. Other modifications were made to expand the applicability of the code and to permit the correlation of chemical structure with a wide variety of biological actions.[4] The inorganic chemistry code is entirely new.[5]

A General Biological Code has been developed by the Biological Codification Panel of the Chemical-Biological Coordination Center and is now available.

As previously mentioned the present code was devised primarily to permit the use of punched cards in the correlation of chemical structure with biological action. Machine methods are especially applicable to the selection of all compounds possessing one or more characteristics in common whereas location of a specific compound is more easily accomplished by hand methods.* For this reason, a code which uniquely defines each compound is not considered necessary.

The present code linearly describes a compound by listing the constituent groups, both functional and nonfunctional. Constituent groups are atoms or groups of atoms which may be identified as units and are described by code designations containing alphabetic or numeric characters. The code for a compound lists the constituent groups present in numeric and alphabetic sequence. Specific rules with examples for assigning code designations to a compound are found in detail in Rules and Directions for Coding Compounds (pp. 8-28), and a list of coded compounds is included (Appendix B, pp. 83-96).

The code designations assigned to the constituent groups are given in the List of Group Numbers (pp. 29-72). The first character of the code number designates the family to which the group belongs. The second and third characters of the code identify the particular structure within the family, and a fourth digit denotes the number of times the group occurs in the compound or ion. A family is defined as an aggregation of chemical groups having certain characteristics in common (See List of Families, Table I, p. 6).

In Division I or the "organic" section of the code (p. 10, Sec. 5), the families are listed in the order of decreasing complexity with respect to the number of elements in the group, proceeding

* Appendix A (pp. 73-82) presents general information on the machines used and the methods of employing the code as an introduction for those unfamiliar with machine methods.

from Family 0-- which contains carbon, hydrogen, nitrogen, oxygen, sulfur and halogen to Family Ø--* which contains only carbon and hydrogen. Generally, two families are used for each combination of elements, one for the noncyclic groups and the other for the cyclic groups. To give preference to functional groups, the noncyclic family precedes the corresponding cyclic family for each combination of elements. An exception was made to this order in the case of Families N-- and Ø-- containing carbon (and hydrogen) to place ring structures before open chain structures.

In the part of the code designated for the coding of "organoheteroid" and "inorganic" groups, assignment of the family designation follows a different plan from that used in the "organic" part of the code. With the exception of Family Q--, the family designation indicates the relationship of the group or element to the remainder of the molecule.

An element (other than C, H, N, O, S or X) attached directly to carbon is coded in Family P--, Division II (p. 24, Sec. 6). The specific element and its combining power are described by the second and third characters of the code designation.

The "inorganic" part of the code, Division III, contains Families Q-- to V--. Family Q-- (p. 25, Sec. 7.5) applies to ring structures containing no carbon. The size of the ring and the number of elements present are indicated by the second and third characters of the code designation. Family R-- (p. 26, Sec. 7.6) designates simple cations and central elements of cations or of neutral molecules and Family T-- (p. 26, Sec. 7.7) simple anions and central elements of anions or of neutral molecules. The basis for assigning central elements of neutral molecules to Family R-- or T-- is described in the Rules and Directions for Coding Compounds (p. 26, Sec. 7.6 and 7.7). The specific element and state of oxidation of the element are described by the second and third characters of the code designation. Groups coordinated to Families R-- and T-- are given code designations in Families S-- and U--, respectively, whereas groups coordinated to Family P-- may appear in either Family S-- or U-- depending upon the character of the P element. Solvate molecules which are associated but not chemically coordinated with a compound are placed in Family V--.

Compounds of indeterminate structure are coded in Family Z--.

As this code does not designate the location of the groups in organic compounds, those containing the same constituent groups have the same code. This includes position isomers and certain other isomers which have the same constituent groups as defined by the code.

Examples: o-$C_6H_4(NO_2)_2$, m-$C_6H_4(NO_2)_2$, p-$C_6H_4(NO_2)_2$

686.2-NYR.1 (686 = RNO_2, R is an aromatic carbocyclic ring; NYR = benzene ring)

$CH_3CH_2COOC_2H_5$, $CH_3COOC_3H_7$

H32.1-Ø7Z.1-Ø89.1 (H32 = RCOOR', R and R' are alicyclic or aliphatic; Ø7Z = 3 carbons in a saturated chain; Ø89 = 2 carbons in a saturated chain)

During the development of the code, the general policy of leaving space for future expansion was consistently followed. Groups which subsequently assume prominence may be assigned numbers in their proper family. Families W--, X-- and Y-- have not been utilized and may be assigned if the need arises.

In addition to recording the structure of a chemical compound, the code also furnishes a method for filing compounds in an organized fashion. An examination of the sequence of the List of Group Numbers (pp. 29-72) shows the order in which the compounds fall in such a file. The original code developed by Frear et al. has been so used in classifying approximately 10,000 organic insecticides and fungicides and is stated to have proved satisfactory for this purpose.[1]

Comments, suggestions and criticisms concerning the Chemical Code will be welcomed. They should be addressed to the National Research Council, Chemical-Biological Coordination Center, 2101 Constitution Avenue, N.W., Washington 25, D.C.

* Ø is used throughout the code to designate the letter O and to distinguish it from zero.

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(4) J.A. Morgan and D.E.H. Frear, J. Chem. Education, 24,58-61 (1947).

(5) J.C. Bailar, Jr., K.F. Heumann and E.J. Seiferle, ibid, 25,142-144 (1948).

RULES Sec. 1 to 4

RULES Sec. 5

RULES Sec. 6 to 7

(CH)NOSX (CH)NOS

CNOS(Z) (CH)NSX

(CH)NOX

(CH)NO

CNO(Z) (CH)NS

CNS(Z)

COS(Z) (CH)NX (CH)OX

TABLE I

LIST OF FAMILIES

* This includes fragments of heterocyclic rings containing a part of the group outside of the ring (See p. 20, Sec. 5.75).

TABLE II

SYMBOLS

M = any cation or metal

m = small whole number

n = small whole number

0 = zero (in group numbers)

ø = letter O (in group numbers)

R = a carbon structure in which C is attached to the balance of the structure as indicated. R', R'', etc. may or may not be the same as R.

X = halogen (F, Cl, Br, I)

x = small whole number

Z = elements other than C, H, N, O, S or X. (In the rare cases in which X occurs in a cyclic structure, it is considered a Z element).

7+ = ring containing 7 or more members

: = double bond

RULES AND DIRECTIONS FOR CODING COMPOUNDS

DEFINITIONS

1. DEFINITION OF STRUCTURES

1.1 A noncyclic structure is a collection of atoms linked together in an open branched or unbranched chain.

1.11 An aliphatic structure is a collection of one or more carbon atoms linked together in an open branched or unbranched chain.

1.2 A cyclic structure is a collection of atoms linked together to form a closed ring.

1.21 An isocyclic structure is a collection of atoms of the same kind linked together to form a closed ring or rings.

1.22 A carbocyclic structure is an isocyclic structure composed of carbon atoms.

1.23 A heterocyclic structure is a collection of atoms of more than one kind linked together to form a closed ring.

1.24 An aromatic structure is a collection of atoms linked together to form a closed ring with resonating double bonds.

1.25 An alicyclic structure is a collection of carbon atoms linked together to form a closed ring which does not contain resonating double bonds.

1.26 A spiro structure is one in which a single atom is the only common member of two rings.

1.27 A fused structure is one containing two or more rings in which adjacent rings share two or more atoms.

1.28 A chelate structure is a collection of atoms formed into a ringlike structure by the establishment of a coordinate covalence.

1.3 A coordinate structure is one which is held together by valence forces which are predominantly covalent as contrasted with ionic. It may be thought of as a "central" atom about which "coordinating" atoms, molecules or ions are clustered.

2. DEFINITION OF GROUPS - A group is a specific combination of atoms which are identified as a unit. A group is not necessarily a functional unit but has been selected for convenience in classification and correlation.

2.1 "Organic" groups - An "organic" group is a combination of linked atoms of which carbon may be one as defined below:

2.11 Groups containing only carbon (and hydrogen) which are the basic structures common to most organic compounds. Examples: ethyl, propyl, phenyl.

2.12 Groups in which carbon is the central element to which are linked one or more of the elements N, O, S or halogen. Examples: ureas, acyl halides, carboxyl groups.

2.13 Groups in which carbon does not itself occur but which must be attached to a group containing carbon in order to partake of organic characteristics. Examples: nitro, amino, chloro.

2.14 For the purposes of this codification system, carbon and the following compounds are not coded as "organic": oxides of carbon, CS_2, $(CN)_2$, $(CNS)_2$ and CNX. All other groups containing carbon are given an "organic" code designation, e.g., metallic carbonates and cyanides are coded as derivatives of carbonic and hydrocyanic acids, respectively.

2.2 "Organoheteroid" groups - An atom other than carbon, hydrogen, nitrogen, oxygen, sulfur or halogen linked directly to carbon is an "organoheteroid" group.

2.3 "Inorganic" groups - In general, an "inorganic" group is one which does not contain carbon. In addition, free carbon and the carbon in oxides of carbon, CS_2, $(CN)_2$, $(CNS)_2$ and CNX are classified as "inorganic". Organic groups which are attached to inorganic compounds as coordinating groups or solvate molecules are given appropriate numbers to express their coordinate or solvate characteristics as well as the requisite numbers in Division I to define their organic structure. Structures classified as "inorganic" are described below:

2.31 Single atoms and molecules consisting of two or more atoms of the same element. Examples: Hg, H_2, S_8.

2.32 Single atoms with a positive charge (simple cations). Examples: Na^+, Al^{+3}.

2.33 Single atoms with a negative charge (simple anions). Examples: Cl^-, P^{-3}.

2.34 Covalent molecules having a central atom to which several other atoms or groups, either like or unlike, are coordinated. Example: $[Co(NO_2)_3(NH_3)_3]$.

2.35 Complex cations which are like the molecules described in 2.34 but possessed of a net positive charge. Example: $[Co(NH_3)_6]^{+3}$.

2.36 Complex anions which are like the molecules described in 2.34 but possessed of a net negative charge. Example: $[Au(CN)_2]^-$

2.37 Various combinations of 2.34, 2.35 and 2.36 in which a molecule or ion contains two or more "central" atoms linked together by a coordinating group or groups. Examples: P_2O_5, $S_2O_7^{-2}$.

2.38 Molecules or ions containing two "central" atoms linked directly to each other. Examples: $S_2O_6^{-2}$, N_2H_4, H_2O_2.

2.39 Compounds containing metals only. Examples: Cu_5Zn_8, $AgCd_3$.

3. DEFINITION OF A FAMILY - A family is an aggregation of chemical groups having certain characteristics in common.

CLASSIFICATION PROCEDURES

4. GENERAL

4.1 The basis for this classification system is the assignment of code designations (group numbers) to component parts of chemical compounds. The component parts are the groups as defined in Sec. 2, and the group numbers are assigned according to the procedure to be detailed in sections to follow. The group numbers for any given compound are arranged in the order of numbers first and letters second. These are separated by dashes for clarity. Example: 174.1-65I.1-H74.1-NYR.1-ø89.1-ø99.2-RB6.1-RGø.1-U63.3.

4.11 The families of groups constitute four main divisions:

Division I.	Families 0-- to ø--, "organic" groups.
Division II.	Family P--, "organoheteroid" groups.
Division III.	Families Q-- to V--, "inorganic" groups including organic coordinate and solvate molecules.
Division IV.	Family Z--, indeterminate structures.

4.12 Chemical compounds may contain groups which are classified in one or more of these divisions, and consequently, in several families. For example, C_2H_5OH contains only organic groups, and both of these fall in Division I. $(C_2H_5)_3PO_4$, on the other hand, contains organic and inorganic groups, which are classified in Divisions I and III, while NaCl contains only inorganic groups, which are classified in Division III only.

RULES Sec. 1 to 4

RULES Sec. 5

RULES Sec. 6 to 7

(CH)NOSX (CH)NOS

CNOS(Z) (CH)NSX (CH)NOX

(CH)NO

CNO(Z) /CH)NS

CNS(Z)

COS(Z) (CH)NX (CH)OX

4.13 A certain few groups appear in both Divisions I and III. These are mainly groups made up of the elements N, O, S or halogen. In Division I, for example, designations for sulfate, nitrate and other radicals are found. These designations are to be used only when the radicals in question are attached to a structure containing carbon. When they are not so attached, they are classified in Division III as inorganic groups.

4.2 Families 0-- to ø-- include all of the "organic" groups. These families are arranged according to the number of different elements present in the groups within the families. All groups containing nitrogen, oxygen, sulfur and halogen (in addition to carbon and hydrogen) comprise Family 0--. Example: bromosulfonamide group, 043. Family 1-- contains those groups having nitrogen, oxygen and sulfur (in addition to carbon and hydrogen). Example: thiocarbamate, 125. Other families follow in order of decreasing complexity. Certain elemental combinations are classified in two families, the cyclic groups being separated from the noncyclic. Example: Noncyclic groups containing nitrogen and oxygen (in addition to carbon and hydrogen) are classified in Family 6-- while cyclic structures containing carbon, nitrogen and oxygen are classified in Family 7--.

4.3 In the "organoheteroid" Family P--, the "organohetero" elements are classified according to their combining power (See Sec. 6.1).

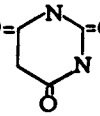
4.4 In Family Q-- (cyclic structures containing no carbon), the group numbers are assigned according to the size of the ring and the number of elements in the ring (See Sec. 7.5).

4.5 In the "inorganic" Families R-- and T--, the individual atoms are classified according to their oxidation state (See Sec. 7.2).

4.6 In Families S--, U-- and V--, groups may contain two or more kinds of atoms which function as units. These may be either organic or inorganic (See Sec. 7.8 and 7.9).

4.7 In Family Z--, a number of indeterminate structures such as proteins, polysaccharides and polymers are designated.

4.8 In all families, the numbers assigned to the individual groups are found in the List of Group Numbers (pp. 29-72). The group numbers consist of four numbers or letters: the first is the family designation; the second and third identify the particular structure within the family; and the fourth designates the number of such groups which occur in the compound (See Sec. 6.2 and 7.4 for exceptions). The fourth digit may be any number from 0 to 9. Zero designates an indeterminate number of groups, 1 to 8 corresponds to the number of groups present, and 9 indicates 9 or more groups. The fourth digit has been separated from the remainder of the code designation by a decimal point, but this convention is entirely optional. In Families P--, R-- and T--, 12 and 11 have frequently been used in the code designations in addition to numbers with a single digit. In order to avoid confusion, 12 and 11 are enclosed in parentheses when used in this manner.

4.9 In coding compounds, the first group encountered in the List of Group Numbers which codes a part of the compound is used. For example, NH_2COOCH_3 is coded as 637.1-ø99.2 and not as F5M.1-H32.1-ø99.2 (637 = $H_2NC(:O)OR$; ø99 = C_1; F5M = RNH_2, R is alicyclic or aliphatic; H32 = $RC(:O)OR'$, R is alicyclic, aliphatic or H, R' is alicyclic or aliphatic). Barbituric acid  is coded as 623.1-GFB.1 and not as 625.1-GFB.1-H5I.2 (623 = $HC(:O)NHC(:O)NHC(:O)H$, GFB = hexahydropyrimidine ring, 625 = $H_2NC(:O)NH_2$, H5I = -C(:O)- (nonketonic)).

5. CODING OF "ORGANIC" GROUPS

5.1 Noncyclic structures containing only carbon (and hydrogen).

5.11 Noncyclic carbon chains are coded according to the total number of carbon atoms occurring together without interruption by some other element and according to their degree of saturation.

5.12 The degree of branching does not affect the classification. 2-Methylpropane and butane are coded as ø7R.1. In the compound $(CH_3)_2CHCH_2\underset{CH_3}{C}HCH_2\underset{CH_2CH_3}{C}HCH_3$, eleven carbon atoms are connected; the code number is therefore ø5I.1. In the compound $(CH_3)_2CHCH_2CH_2NHCH_2CH_3$, the carbon chain is interrupted by the nitrogen atom. The two chains are coded as ø7I.1 (C_5 saturated) and ø89.1 (C_2 saturated).

5.13 Carbon chains attached to cyclic structures are coded separately. For example, $C_6H_5C_3H_7$ is coded as NYR.1-ø7Z.1 and $C_6H_5CH_3$ as NYR.1-ø99.1 (NYR = benzene ring, ø7Z = C_3 saturated, ø99 = C_1).

5.14 Isolated carbon atoms are given the C_1 number (ø99). For example, $-CH_3$ in toluene is coded as ø99.1. This also applies to carbon atoms occurring in complex groups. For example, CH_3CH_2NC, ethyl isocyanide, is coded F78.1-ø89.1-ø99.1; H_2NCONH_2, urea, is coded 625.1-ø99.1 (F78 = HNC, ø89 = C_2 saturated, 625 = $H_2NC(:O)NH_2$).

5.15 Specific code numbers (ø6K-ø99) are assigned to each degree of unsaturation in noncyclic hydrocarbon groups containing up to and including 6 carbon atoms. Examples: $CH_3CH_2CH_3$ is ø7Z.1; $CH_3CH{:}CH_2$ is ø7Y.1; $CH_3C{:}CH$ is ø7W.1; and $CH_2{:}C{:}CH_2$ is ø7X.1.

5.16 Unsaturation in noncyclic hydrocarbon groups containing 7 to 20 or more carbon atoms is indicated in a less detailed manner (ø28-ø6I).

5.2 Noncyclic polyelement structures.

5.21 In listing the noncyclic polyelement groups in the List of Group Numbers, both R and H have been used to delineate the group. If no R or carbon atom appears in the group as listed, at least one of the H's must be replaced by a structure containing carbon, otherwise the compound is inorganic. For example, unsubstituted hydroxylamine is not coded by code designation 677 (H_2NOH) but by code designations in Families T-- and U--.

5.211 R has been used only when an R structure must be present in the specific position shown. R may be H as stated in the List of Group Numbers in the following instances: aliphatic secondary and primary amides (65C, 65H, 65I and 65L), carboxylic acids and esters (H32, H37, H38, H39 and H42), aldehydes (H5D) and primary alcohols (H8M). Since these groups contain a carbon as an integral part of the group, this practice allows coding of the first member of the series by the same code designation as those in which a hydrogen has been replaced by an aliphatic carbon. For example, the amide group in formamide ($HCONH_2$) is coded as 65L.1 (65L = $RC(:O)NH_2$, R is alicyclic, aliphatic or H).

5.212 H is replaceable by a metal, by R except in the cases listed in the next paragraph, and in certain instances, by a nonmetal as is shown in Sec. 5.222. For example, the sulfonate groups in $C_6H_5SO_3H$, $C_6H_5SO_3Na$ and $C_6H_5SO_3CH_3$ are all coded as A42.1 (HSO_3H).

H cannot be replaced by R when the group so formed containing R becomes thereby a structure which is described by a code designation preceding that of the corresponding group containing H. Thus specific listings of the R derivatives have been made in order to separate into different categories groups which would otherwise fall under the same code designation. Carbamic acid esters (630-637) are separated from carbamic acids (639), carboxylic acid esters (H26-H39) from carboxylic acids (H40-H48), ketones (H50-H59) from aldehydes (H5B-H5G), ethers (H61-H69) from phenols and alcohols (H72-H8Z), thiones (J51) from thioaldehydes (J55), and sulfides (J65-J66) from thiols (J72). Likewise, primary, secondary and tertiary derivatives are given different code designations in the following cases: sulfonamides (170-177), carbamic acid esters (630-637), amides (650-65L), nitroamines (664-665), nitrosoamines (667-668), thioamides (850-853), amines (F50-F5M) and alcohols (H81-H8R). Examples: $CH_3C(:O)CH_3$ is coded as H54.1-ø7Z.1; $CH_3CH_2C(:O)H$ as H5D.1-ø7Z.1 (H54 = $RC(:O)R'$, R and R' are alicyclic or aliphatic; ø7Z = C_3 saturated;

RULES Sec. 5

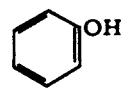
RULES Sec. 6 to 7

(CH)NOSX (CH)NOS CNOS(Z) (CH)NSX (CH)NOX (CH)NO CNO(Z) /CH)NS CNS(Z)

H5D = RC(:O)H, R is alicyclic, aliphatic or H). $(C_2H_5)_2NH$ is coded as F5D.1-ø89.2; $C_2H_5NH_2$ as F5M.1-ø89.1 (F5D = RR'NH, R and R' are alicyclic or aliphatic; ø89 = C_2 saturated; F5M = RNH_2, R is alicyclic or aliphatic).

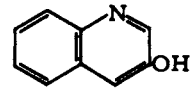
5.213 The nature of R to which certain of the most commonly occurring groups are attached is definitely specified in order to bring about a greater separation of the types of compounds within these categories. The nature of R is specified in the following groups: amides (646, 650-65L), nitro compounds (685-687), amines (F50-F5M), carboxylic acid esters (H26-H38), carboxylic acids (H40-H42), ketones (H50-H57), aldehydes (H5B-H5D), ethers (H61-H67), phenols (H72-H74), alcohols (H81-H88, H8A-H8G, H8K-H8M) and halo compounds (L22-L27, L32-L37, L42-L47, L52-L57). To permit the coding of compounds in which the structure of R is not specifically known, code designations with R unspecified have been added at the end of each of the above groups. Examples of coding of -OH group:

ROH:



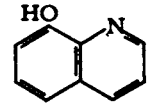
H74.1

(R is aromatic monocarbocyclic)



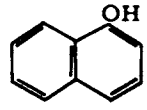
H72.1

(R is aromatic heterocyclic)



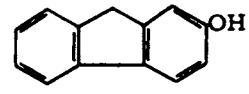
H74.1

(R is aromatic monocarbocyclic)



H73.1

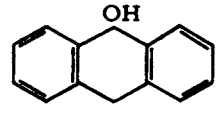
(R is aromatic polycarbocyclic)



H73.1

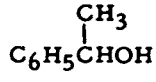
(R is aromatic polycarbocyclic)

R—CHOH:



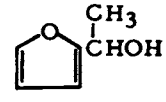
H8A.1

RR'CHOH:



H8G.1

(R is aromatic carbocyclic, R' is alicyclic or aliphatic)



H8F.1

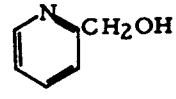
(R is heterocyclic, R' is alicyclic or aliphatic)

RCH_2OH:

CH_3CH_2OH

H8M.1

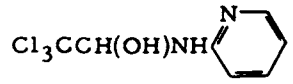
(R is alicyclic, aliphatic or H)



H8K.1

(R is heterocyclic)

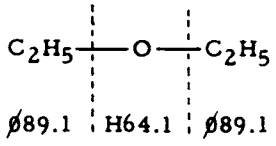
<u>>CHOH (attached to an element other than carbon):</u>



H8I.1

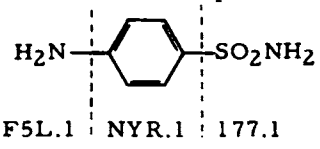
5.214 Since R is a variable structure, it should be appreciated that the interpretation of its significance must be made compatible with its place in the List of Group Numbers. For example, R of an ether (ROR') could not be R''C(:O)- for the resulting structure (R''C(:O)OR') would be an ester.

5.22 In splitting compounds into component groups for coding, the groups are ordinarily separated at the point of attachment to a carbon atom. Examples:



ø89.1 | H64.1 | ø89.1

(Coded as H64.1-ø89.2)

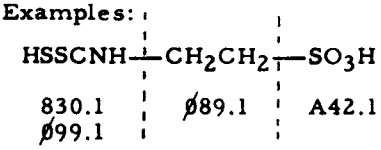


F5L.1 | NYR.1 | 177.1

(Coded as 177.1-F5L.1-NYR.1)

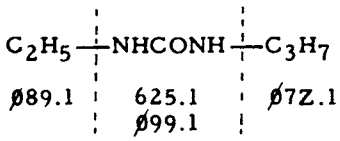
(H64 = ROR', R and R' are alicyclic or aliphatic; ø89 = C_2 saturated; 177 = HSO_2NH_2; F5L = RNH_2, R is aromatic carbocyclic; NYR = benzene ring)

5.221 Certain groups, such as urea, carbamate, etc., contain one or more single carbon atoms as integral parts of the group. Such groups are separated for coding at their point of attachment to other carbon atoms, and the isolated carbon atoms are given code number ø99.1 (See Sec. 5.14). Examples:



830.1 ø99.1 | ø89.1 | A42.1

(Coded as 830.1-A42.1-ø89.1-ø99.1)

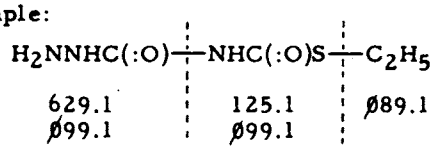


ø89.1 | 625.1 ø99.1 | ø7Z.1

(Coded as 625.1-ø7Z.1-ø89.1-ø99.1)

(830 = $H_2NC(:S)SH$, A42 = HSO_3H, ø89 = C_2 saturated, ø99 = C_1, 625 = $H_2NC(:O)NH_2$, ø7Z = C_3 saturated)

5.222 In order to permit the coding of groups which are not specifically designated in the List of Group Numbers, an exception may be made to the rule that compounds are broken into groups for coding at the point of attachment to a carbon atom. Under these conditions, H may be replaced by a group other than R or M. This procedure should not be used unless the group under consideration can not be found in the List of Group Numbers. Example:



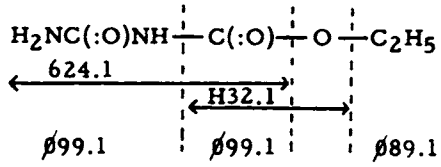
629.1 ø99.1 | 125.1 ø99.1 | ø89.1

(Coded as 125.1-629.1-ø89.1-ø99.2)

(125 = $NH_2C(:O)SH$, 629 = $HC(:O)NHNH_2$, ø89 = C_2 saturated, ø99 = C_1)

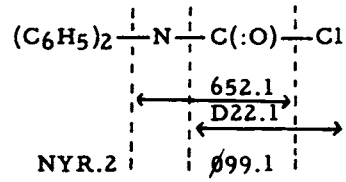
In this example an H of $HC(:O)NHNH_2$ is replaced by N for purposes of coding.

5.223 In cases where this procedure results in an uncoded fragment which is not a recognizable group (Sec. 2.11, 2.12, 2.13), the minimum portion of the previously coded structure adjacent to the uncoded fragment is included with it to designate adequately the uncoded residue. Examples:



(Coded as 624.1-H32.1-ø89.1-ø99.2)

(624 = $H_2NC(:O)NHC(:O)H$; H32 = RC(:O)OR', R is aliphatic, alicyclic or H, R' is aliphatic or alicyclic; ø89 = C_2 saturated; ø99 = C_1)

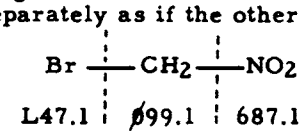


(Coded as 652.1-D22.1-NYR.2-ø99.1)

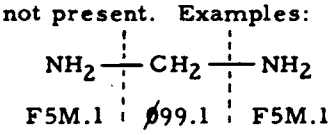
(652 = HC(:O)NRR', R is aromatic carbocyclic, R' is aromatic carbocyclic, alicyclic or aliphatic; D22 = HC(:O)Cl; NYR = benzene ring; ø99 = C_1)

It should be noted in both of the examples given above the carbonyl group has been double coded. In the first example, the first group encountered in the List of Group Numbers which codes a portion of the structure is an acyl urea (624); $-OC_2H_5$ then remains as an uncoded fragment. It has already been pointed out in Sec. 5.214 that the interpretation of R must be made compatible with the structure described in the List of Group Numbers. In this case, the fragment is not an ether and a portion of the previously coded structure is included to describe the structure adequately. Inclusion of the carbonyl group is the minimum portion which permits an appropriate coding of the $-OC_2H_5$ fragment. Likewise in the second example, the uncoded -Cl is not adequately coded by L37 (L37 = RCl, R is alicyclic or aliphatic). For this reason, the carbonyl group is double coded and the group is characterized as an acyl halide.

5.224 When there is no group listed which codes all of the groups attached to a single carbon atom, then each group attached to the carbon atom is coded separately as if the other group were not present. Examples:



(Coded as 687.1-L47.1-ø99.1)



(Coded as F5M.2-ø99.1)

(687 = RNO_2, R is alicyclic or aliphatic; L47 = RBr, R is alicyclic or aliphatic; ø99 = C_1; F5M = RNH_2, R is alicyclic or aliphatic)

5.23 A distinction is made between certain groups which may be attached to two or more separate (and possibly different) groups on the one hand, and those which by definition must be attached by a double bond to the same group as indicated by R:. Examples:

$C_6H_5CH{:}NNH_2$	$C_6H_5CH_2NHNH_2$
F30.1-NYR.1-ø99.1	F35.1-NYR.1-ø99.1

(F30 = $R{:}NNH_2$, NYR = benzene ring, ø99 = C_1, F35 = H_2NNH_2)

No attempt has been made to distinguish in all instances between a double and a single bond attachment to carbon. When a separate group is not listed for the structure containing a double bond, then two H's or R,R' in the corresponding saturated structure may be replaced by R:. Examples:

$CH_3CONHN{:}CHC_6H_5$	$(CH_3)_2C{:}NN{:}C(CH_3)_2$
629.1-NYR.1-ø89.1-ø99.1	F30.1-ø7Z.2

(629 = $HC(:O)NHNH_2$, NYR = benzene ring, ø89 = C_2 saturated, ø99 = C_1, F30 = $R{:}NNH_2$, ø7Z = C_3 saturated)

$CH_2{:}C{:}O$ $CH_3CH(C_6H_5){:}COH$

H54.1-ø88.1 H87.1-NYR.1-ø7Y.1

(H54 = RC(:O)R', R and R' are alicyclic or aliphatic; ø88 = C_2 with 1 double bond; H87 = RR'R''COH, R,R',R'' are aromatic carbocyclic and alicyclic or aliphatic; NYR = benzene ring; ø7Y = C_3 with 1 double bond)

5.24 Multiple linkages between atoms (except carbon to carbon) are not coded.

5.3 Monocyclic structures containing only carbon.

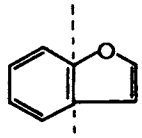
5.31 Cyclic structures containing only carbon atoms in the ring are coded in Family N--. Examples:

NZ9.1

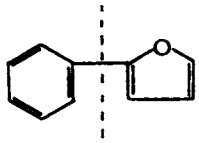
NYR.1

5.32 In monocyclic hydrocarbon structures containing six members or less, all states of saturation are designated by specific group numbers. Examples: benzene (NYR), cyclohexadiene (NYM) and cyclohexane (NYK). In monocyclic hydrocarbon structures with more than six members, three states of saturation are designated, namely, complete saturation (NY2), unsaturation other than maximum (NY5) and maximum conjugated unsaturation (NY9). Maximum conjugated unsaturation is defined as the maximum number of unsaturated linkages possible when no double bonds are adjacent.

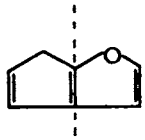
5.33 All cyclic hydrocarbon structures fused (attached at more than one point) to a heterocyclic ring are separated for coding. The appropriate group number is assigned to each ring structure. Separate code designations are listed for fused and unfused six-membered carbocyclic rings, but other carbocyclic rings are coded by the same designations regardless of whether they are fused or unfused. Examples:



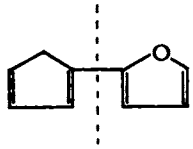
NYI.1 | IP9.1



NYR.1 | IP9.1

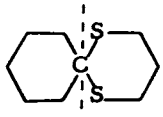


NZ9.1 | IP9.1



NZ9.1 | IP9.1

5.34 Spiro compounds are separated into their component structures for coding. Example:



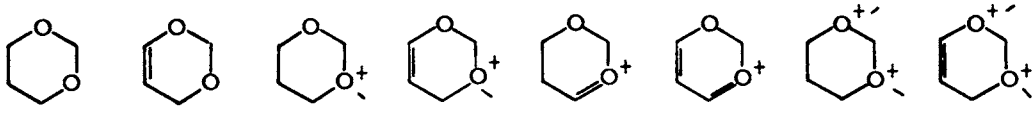
NYK.1 | KF2.1

5.4 Monocyclic polyelement structures (heterocyclic structures).

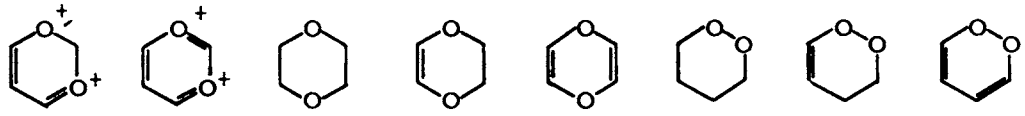
5.41 Ring structures containing one or more of the elements nitrogen, oxygen or sulfur in addition to carbon are coded in the appropriate family as indicated in the List of Group Numbers. For example, a saturated six-membered ring containing four carbon atoms, one nitrogen atom and one sulfur atom is coded in the CNS family as 9I2.

5.42 In heterocyclic structures, the states of saturation are indicated in the same general manner as in the carbocyclic structures. In most cases, three states of saturation are indicated, namely, complete saturation, unsaturation other than maximum and maximum unsaturation. Unsaturation has been more specifically designated for a few frequently occurring ring structures such as C_5N. Maximum

unsaturation of heterocyclic ring structures is defined as the maximum number of unsaturated linkages possible when no double bonds are adjacent and when each element is assigned the valence it possesses in the specific compound under consideration. Examples:



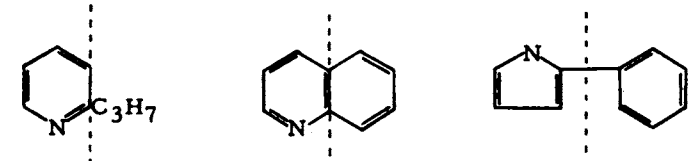
IF2 IF9 IF2 IF5 IF5 IF9 IF2 IF5



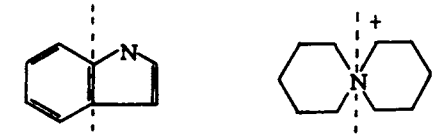
IF5 IF9 IF2 IF5 IF9 IF2 IF5 IF9

(IF2 = C_4O_2, complete saturation; IF5 = C_4O_2, unsaturation other than maximum; IF9 = C_4O_2, maximum unsaturation)

5.43 Heterocyclic units attached to any other structure are coded as separate structures. Because of the frequency of occurrence of C_5N rings, separate code designations are listed for fused and unfused C_5N rings. Other heterocyclic ring structures are coded by the same designations in both the fused and unfused state. Examples:



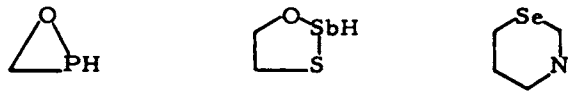
GH9.1 ; 07Z.1 GG9.1 ; NYI.1 GP9.1 ; NYR.1



NYI.1 ; GP9.1 GH2.1 ; GH2.1

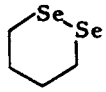
5.44 Elements other than C, N, O, S or X are designated as Z elements. In the rare cases in which X occurs in a cyclic structure, it is considered a Z element. Cyclic structures in which such elements occur are called Z rings. Chelate rings are not considered cyclic structures (See Sec. 5.99). In addition to the group number assigned to the rings as indicated below, the Z elements are assigned group numbers in the "organoheteroid" or "inorganic" families (See Sec. 6.3, 7.65 and 7.75).

5.441 Z rings in which N, O or S also occur (along with carbon) are coded in the appropriate families (2--, 7--, 9--, B--, G--, I-- or K--). Examples:



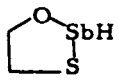
I3K.1 B2K.1 G22.1

5.442 Z rings which contain only carbon and Z elements make up Family M--. Example:

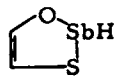


MF2.1

5.443 Unsaturation in Z rings containing carbon is indicated in the same manner as in the other heterocyclic structures. Examples:



B2K.1

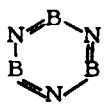


B2R.1

G22.1

G29.1

5.444 Rings containing no carbon are coded in Family Q--. These are inorganic by definition, and no differentiation is made between states of saturation (See Sec. 7.5).

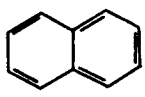


Q62.1

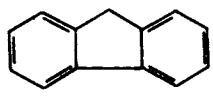
Q51.1

5.5 Polycyclic structures containing only carbon.

5.51 Condensed polycyclic rings containing only carbon in the rings are not broken down for coding, but are given the appropriate number in Family N--. Examples:

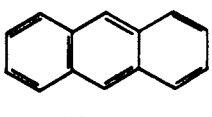


NTR.1

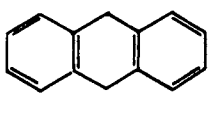


NN9.1

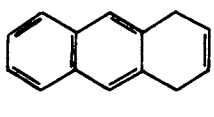
5.52 In the more frequently occurring carbocyclic structures, such as naphthalene, anthracene, etc., the state of saturation is specifically designated by an appropriate group number. In other ring structures, three states of saturation are indicated, namely, complete saturation, unsaturation other than maximum and maximum conjugated unsaturation. Maximum conjugated unsaturation is defined as the maximum number of unsaturated linkages possible when no double bonds are adjacent. Examples:



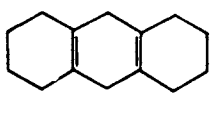
NKI.1



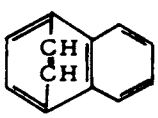
NKH.1



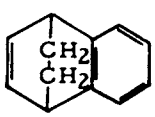
NKH.1



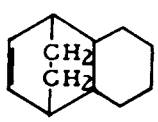
NKD.1



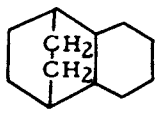
NLI.1



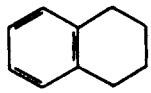
NLE.1



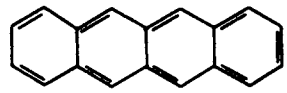
NLE.1



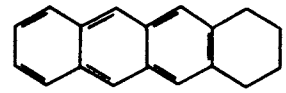
NLB.1



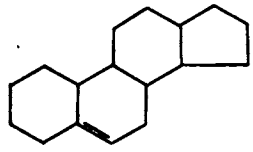
NTN.1



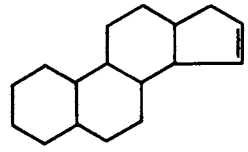
N3I.1



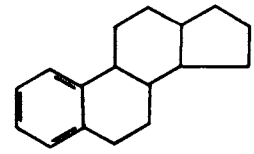
N3E.1



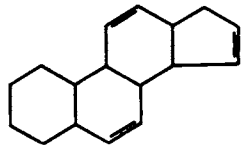
N63.1



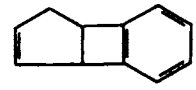
N63.1



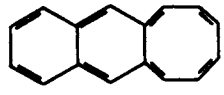
N65.1



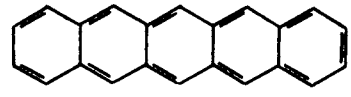
N65.1



NPV.1

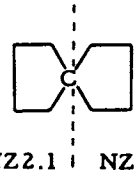


NJR.1

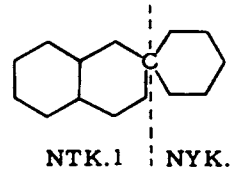


N05.1

5.53 Spiro compounds are separated into their component structures for coding. The common atom is coded as part of each separate unit. Examples:

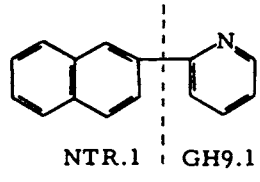


NZ2.1 NZ2.1

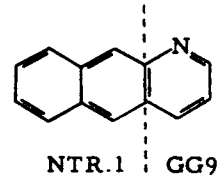


NTK.1 NYK.1

5.54 In multiple ring structures in which a polycyclic hydrocarbon structure is attached to a heterocyclic structure, the two structures are separated for coding. The same group number is assigned to polycyclic rings whether they be fused to other structures or occur independently. Examples:



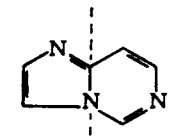
NTR.1 GH9.1



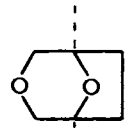
NTR.1 GG9.1

5.6 Polycyclic polyelement structures.

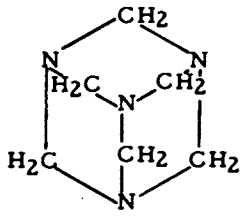
5.61 Multiple ring structures made up of two or more heterocyclic units sharing two or more common atoms are separated for coding. Common atoms shared by two or more rings are coded as part of the least number of rings necessary to describe the complete structure. Examples:



GN9.1 GFD.1

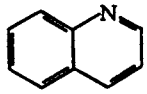


IF2.1 IP2.1

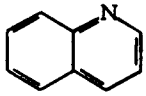


GD2.3

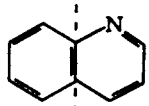
5.62 Unsaturation in polycyclic polyelement structures is coded as in the monocyclic polyelement structures (See Sec. 5.42). When a heterocyclic structure is fused to another heterocyclic structure or to a carbocyclic structure, a resonating, conjugated double bond system is arbitrarily so designated that the maximum number of double bonds possible is shown within each ring. Structure C is to be used in the example below.



A



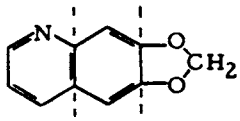
B



NYI.1 GG9.1

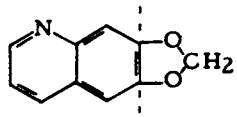
C

In the more complex fused system given below, structure A is used in coding the nitrogen ring whereas structure B is used in coding the oxygen ring.



GG9.1 NYI.1

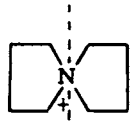
A



IN9.1

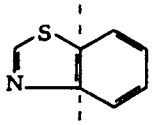
B

5.63 Spiro compounds in which a single heteroatom is shared between two rings are always coded as two separate rings, the common atom being counted in both rings. Example:

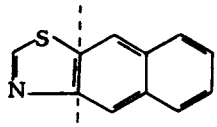


GP2.1 GP2.1

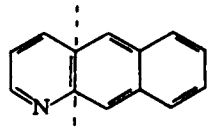
5.64 In multiple ring structures containing a heterocyclic unit fused (attached at more than one point) to a carbocyclic structure, the heterocyclic unit is separated for coding. Examples:



9ø9.1 NYI.1



9ø9.1 NTR.1



GG9.1 NTR.1

The shared double bonds are double coded, i.e., coded as present in both cyclic structures. In some cyclic compounds, there are conjugated double bond systems which do not resonate and are thus fixed as to location in the structure. These are coded according to the appropriate rules (Sec. 5.42 and 5.61).

5.7 Double coding.

In a system of this kind, it is not always possible to make a sharp cleavage between adjacent groups, each of which partakes to some extent of the properties of the other. Many such groups are "double coded", i.e., an atom or group of atoms shared by two structures is considered to be part of both.

5.71 Isolated carbon atoms occurring in groups are coded as C_1 groups (ø99). This convention, which has been mentioned in Sec. 5.14, allows all carbon atoms to be taken into account.

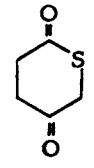
5.72 The carbon atom forming part of a carboxyl group, aldehyde group, carbinol group, etc. is coded separately if attached to cyclic structures (Sec. 5.13) or added to the carbon chain if attached to an aliphatic group. Examples:

CH_3COOH	H42.1-ø89.1	(H42 = RC(:O)OH, R is alicyclic, aliphatic or H; ø89 = C_2 saturated)
C_6H_5COOH	H41.1-NYR.1-ø99.1	(H41 = RC(:O)OH, R is aromatic carbocyclic; NYR = benzene ring; ø99 = C_1)
CH_3CONH_2	65L.1-ø89.1	(65L = RC(:O)NH_2, R is alicyclic, aliphatic or H; ø89 = C_2 saturated)
$C_6H_5CONH_2$	65K.1-NYR.1-ø99.1	(65K = RC(:O)NH_2, R is aromatic carbocyclic; NYR = benzene ring; ø99 = C_1)

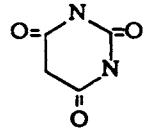
5.73 In cyclic structures which share one or more common atoms (Sec. 5.61-5.64), the shared atom or atoms are counted as belonging to both rings. Many examples have already been given.

5.74 Certain parts of the structure are double coded when it has been found essential to do so to describe the structure adequately (See Sec. 5.223).

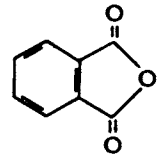
5.75 A group attached to a heteroatom or an atom adjacent to a heteroatom of a heterocyclic structure is considered to contain that atom and adjacent atoms as a component part. This convention applies only to groups lying partially outside of the ring unless a cyclic code designation has been added for the heteroatom in the ring (See Sec. 5.76). Examples:



A20.1-H51.1-KH2.1



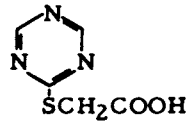
623.1-GFB.1



H23.1-IP5.1-NYI.1

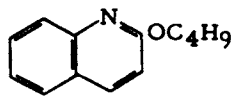
(A20 = HC(:O)SH, H51 = $H_2CC(:O)CH_2$, KH2 = tetrahydrothiapyran ring, 623 = HC(:O)NHC(:O)NHC(:O)H, GFB = hexahydropyrimidine ring, H23 = HC(:O)OC(:O)H, IP5 = dihydrofuran ring, NYI = fused benzene ring)

In heterocyclic compounds containing resonating double bonds, the bonds are always to be coded as part of the aromatic structure; they are not considered to be parts of tautomeric systems involving groups lying outside the rings. Examples:



F50.3-GD9.1-H42.1-J66.1-ø89.1 and <u>not</u> 825.1-F50.1-GD9.1-H42.1-ø89.1

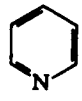
(F50 = R:N; GD9 = triazine ring; H42 = RC(:O)OH, R is alicyclic, aliphatic or H; J66 = RSR'; ø89 = C_2 saturated; 825 = $H_2NC(:NH)SH$)



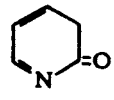
F50.1-GG9.1-H66.1-NYI.1-ø7R.1 and not 649.1-GG9.1-NYI.1-ø7R.1

(F50 = R:N; GG9 = fused pyridine ring; H66 = ROR', R is heterocyclic, R' is alicyclic or aliphatic; NYI = fused benzene ring; ø7R = C_4 saturated; 649 = HC(OR)(:NH))

5.76 Cyclic code designations have been assigned to certain groups which commonly occur as component parts of heterocyclic structures in order to separate the cyclic groups from the corresponding noncyclic groups. In every case, the cyclic designation precedes the noncyclic group in the List of Group Numbers so that no confusion arises regarding which code designation is to be used. The groups thus coded are sultams (166), cyclic tertiary sulfonamides (170), cyclic carbamic acid esters (630), lactams (646), cyclic tertiary amides (650) and thioamides (850), sultones (A36), cyclic quaternary ammonium compounds (F41 and F43), cyclic tertiary and secondary amines (F50, F51 and F5A), cyclic peroxides (H10), lactones (H26), cyclic acetals (H4J), quinones (H50), cyclic ketones (H51), cyclic ethers (H61), cyclic tertiary and secondary alcohols (H81 and H8A), cyclic disulfides (J62) and cyclic sulfides (J65). In some of these groups, a portion of the group lies outside of the ring (amides, lactones, etc.) whereas in others the group is completely within the ring (amines, peroxides, etc.). Examples:

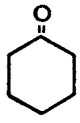


F50.1-GH9.1

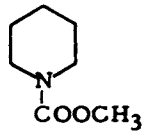


646.1-GH4.1

(F50 = R:N, GH9 = pyridine ring, 646 = RC(:O)NH, GH4 = dihydropyridine ring)



H51.1-NYK.1



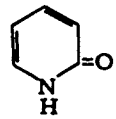
630.1-GH2.1-ø99.2

(H51 = $H_2CC(:O)CH_2$, NYK = cyclohexane ring, 630 = R'-NC(:O)OR, GH2 = piperidine ring, ø99 = C_1)

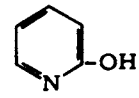
5.8 Unspecified groups - Provision is made for coding unknown or unspecified groups. Unspecified alkyl groups are coded as øZZ, unspecified carbocyclic groups as NZZ, unspecified heterocyclic groups as ZZ0 and unspecified structures containing carbon as ZZA.

5.9 Specific conventions.

5.91 Tautomerism. In compounds which may exist in tautomeric forms, a specific structure must be assigned to the compound before coding. Thus, in keto-enol tautomers, for example, the person using the code must decide whether the compound is a ketone or an alcohol, or exists in both forms, and must assign code numbers accordingly. In the case of certain noncyclic tautomeric forms, e.g., 125, 625, 65A-65L, etc., the same group number is assigned to both tautomeric forms. Examples:



646.1-GH4.1



F50.1-GH9.1-H72.1

(646 = RC(:O)NH; GH4 = dihydropyridine ring; F50 = R:N; GH9 = pyridine ring; H72 = ROH, R is aromatic heterocyclic)

$H_2NC(:O)NH_2$ $H_2NC(:NH)OH$

625.1-ø99.1 625.1-ø99.1

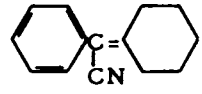
(625 = $H_2NC(:O)NH_2$ or $H_2NC(:NH)OH$, ø99 = C_1)

5.92 Separate numbers are given to certain isomeric structures such as the acylthiocyanates (180) and acylisothiocyanates (181), the cyanates (661) and isocyanates (662), the thiocyanates (861) and isothiocyanates (862) and the nitriles (F75) and isocyanides (F78) (cf. Sec. 5.91).

5.93 In the case of a few groups such as the amines, distinction is made between primary, secondary and tertiary forms (F5-) (See Sec. 5.212).

5.94 In the case of certain of the more commonly occurring groups such as amines and acids, the nature of the carbon structure to which the group is attached is specified in the List of Group Numbers (See Sec. 5.213).

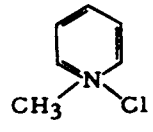
5.95 Carbon to carbon double bonds which are intercyclic or between cyclic and noncyclic structures are coded as ø08. Example:

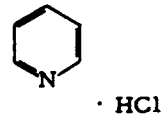


F75.1-NYK.1-NYR.1-ø08.1-ø89.1

(F75 = HCN, NYK = cyclohexane ring, NYR = benzene ring, ø08 = C:C or C:R, ø89 = C_2 saturated)

Ammonium compounds with all four hydrogens on the nitrogen replaced by other groups are coded as quaternary ammonium compounds (F41-F47), but acid salts of amines are coded as amines and acids (See Sec. 7.6 and 7.7 for coding inorganic acids). Examples:





F41.1-GH9.1-ø99.1-T69.1 F50.1-GH9.1-RB6.1-T69.1

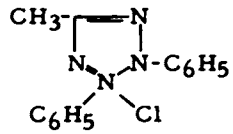
(F41 = RR':N^+, GH9 = pyridine ring, ø99 = C_1, T69 = Cl^{-1}, F50 = R:N, RB6 = H^{+1})

$(CH_3)_4NCl$ $(CH_3)_2NH \cdot HCl$

F46.1-ø99.4-T69.1 F5D.1-ø99.2-RB6.1-T69.1

(F46 = RR'R''R'''N^+; ø99 = C_1; T69 = Cl^{-1}; F5D = RR'NH, R and R' are alicyclic or aliphatic; RB6 = H^{+1})

A special group $>N<^+$ or $\ulcorner\overset{\diagup\diagdown}{N}\urcorner^+$ (F47) has been added to code quaternary ammonium compounds in which an element other than carbon is attached to the quaternary nitrogen atom. Example:



F47.1-GJ9.1-NYR.2-ø99.1-T69.1

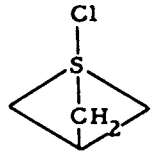
(F47 = $\overset{\diagdown\ \diagup\ +}{\text{N}}$ attached to an element other than carbon, GJ9 = tetrazole ring, NYR = benzene ring, ø99 = C_1, T69 = Cl^{-1})

Hydrogen derivatives of oxonium and sulfonium compounds, as well as those in which three carbon structures are attached to the O or S, are coded as H90 and J90, respectively. Examples:

$(CH_3)_2O \cdot HBr$

H90.1-ø99.2-T49.1

(ø99 = C_1, T49 = Br^{-1})



J90.1-KV2.2-T69.1

(KV2 = thietane ring, T69 = Cl^{-1})

5.97 Group numbers for coding nonketonic carbonyls (H5I) and nonketonic thiocarbonyls (J59) are included to eliminate the necessity of double coding. Examples:

$C_6H_5CONHNHCOC_6H_5$

629.1-H5I.1-NYR.2-ø99.2

(629 = $HC(:O)NHNH_2$, NYR = benzene ring, ø99 = C_1)

Group numbers (H89, H8I and H8R) are used to code nonaromatic hydroxy compounds which contain elements other than carbon or hydrogen attached to the carbinol group. Examples:

H_2NCH_2OH

F5M.1-H8R.1-ø99.1

(F5M = RNH_2, R is alicyclic or aliphatic; H8R = $-CH_2OH$, attached to an element other than carbon; ø99 = C_1)

$H_2NCON[CH(OH)CCl_3]_2$

625.1-H8I.2-L37.6-ø89.2-ø99.1

(625 = $NH_2C(:O)NH_2$; H8I = >CHOH, attached to an element other than carbon; L37 = RCl, R is alicyclic or aliphatic; ø89 = C_2 saturated; ø99 = C_1)

5.98 Alkoxy and aryloxy and the corresponding sulfur derivatives of Si, B, Sb, Te, As, P and Se are coded as esters of inorganic acids (See Sec. 4.12) whereas the analogous derivatives of elements in Family R-- (See Sec. 7.64) are coded as derivatives of phenols, alcohols or thiols. Examples:

C_2H_5OK

H8M.1-ø89.1-RDø.1

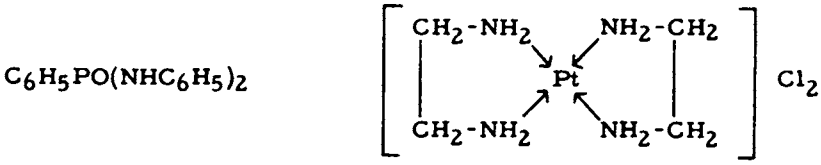
(H8M = RCH_2OH, R is alicyclic, aliphatic or H; ø89 = C_2 saturated; RDø = K^{+1})

$(C_6H_5O)_3AsO$

NYR.3-T1J.1-U63.4

(NYR = benzene ring, T1J = As^{+5}, U63 = :O or -O-)

A similar distinction is made between nitrogen derivatives of the elements listed above and nitrogen derivatives of elements in Family R--. Examples:



NYR.3-PJ1.1-U32.2-U63.1

(NYR = benzene ring, PJ1 = P^5, U32 = $-NH_2$, U63 = :O or -O-)

F5M.4-ø89.2-RL7.1-S3B.2-T69.1

(F5M = RNH_2, R is alicyclic or aliphatic; ø89 = C_2 saturated; RL7 = Pt^{+2}; S3B = $R(NH_2)_2$, bidentate; T69 = Cl^{-1})

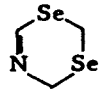
5.99 Chelate rings are coded as open chain structures. The coding of a chelate compound is shown in Sec. 5.98.

6. CODING OF "ORGANOHETEROID" GROUPS

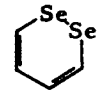
6.1 "Organoheteroid" groups are elements other than carbon, hydrogen, nitrogen, oxygen, sulfur or halogen linked directly to carbon as defined in Sec. 2.2. They are assigned group numbers in Family P--. In this family, the groups are designated by a series of numbers, the second and third digits of which identify the specific combining powers of each element. Combining power is defined as the number of electrons which the atom in question furnishes for sharing or transfers to other atoms. The fourth digit indicates the number of such groups present in the compound. For example, the group number for Hg in $C_6H_5HgNO_3$ is PC5.1; the As in $(C_6H_5)_2AsO_2H$ is P1J.1 and in $(C_6H_5)_2AsH$ is P1L.1; SiC is ø99.1-PP1.1; and Cu_2C_2 is ø86.1-P7ø.2 (PC5 = Hg^2, P1J = As^5, P1L = As^3, ø99 = C_1, PP1 = Si^4, ø86 = C_2 with triple bond, P7ø = Cu^1).

6.2 In a chain of two or more like "organohetero" elements linked together, a special combination of the second and third digit in the group number is assigned; in such cases, the fourth digit indicates the number of atoms linked together. For example, the group number for the chain of As atoms in $(CH_3)_2AsAs(CH_3)_2$ is P1(11).2; the group number for the chains of As atoms in $CH_3As{:}AsCH_2CH_2As{:}AsCH_3$ is likewise P1(11).2.

6.3 In heterocyclic rings containing Z elements (See Sec. 5.44), the Z elements are given appropriate group numbers in Family P-- if they are directly attached to carbon. If two or more like Z atoms occur together, they are assigned a group number for a chain as indicated in Sec. 6.2. It should be noted that this is another example of double coding. Examples:



F50.1-G29.1-PøN.2



MF9.1-Pø(11).2

(F50 = R:N; G29 = 6-membered CNZ ring, maximum unsaturation; PøN = Se^2; MF9 = C_4Z_2 ring, maximum unsaturation; Pø(11) = Se chain)

7. CODING OF "INORGANIC" GROUPS

7.1 General.

7.11 Elements are considered to be "inorganic" (Sec. 2.3) when they are not specifically classified as "organic" or "organoheteroid" and are assigned group numbers in Families Q--, R--, S--, T--, U-- or V--.

7.12 It is recognized that it is not always possible to distinguish between a covalent and an ionic bond. In such cases, the compound is coded as if the bond were ionic.

7.2 Oxidation states of "inorganic" groups. The group number assigned to an "inorganic" element is determined by its oxidation state. The following rules apply:

7.21 The oxidation state of an atom of a free element is zero. This is true whether the atom is in the monatomic or in the polyatomic state. Examples: He, Cl_2, O_3, S_8.

7.22 The oxidation state of elements in an intermetallic compound is considered to be zero.

7.23 The oxidation state of an atom which is a member of a chain need not be calculated as it is not used in this scheme.

7.24 The oxidation states of elements not included in 7.21 and 7.22 are calculated in the conventional way, i.e., by assuming that enough shared electrons to fill the outer shell of the more electron-attracting atom belong to that atom. If the oxidation state of an element is indeterminate or if the ratio of elements in the compound is not in accord with stoichiometric principles, the element is assigned the code number indicating zero or indeterminate values. Example: FeAsS is R9R.1-T1Ø.1-TNP.1 (R9R = Fe°, T1Ø = As°, TNP = S°).

7.25 The oxidation state of a simple ion is the charge on the ion.

7.3 The order of increasing electronegativity is taken as Si, B, Sb, Te, As, P, Se, I, S, C, Br, Cl, N, O, F. Examples: In $(ClO)^-$, Cl is considered to be positive (T67.1) with respect to O (U63.1); N in NO is considered to be positive (TGD.1) with respect to O (U63.1).

7.4 The fourth digit in "inorganic" group numbers is assigned as follows:

7.41 In simple ions, the fourth digit is one since by definition only one atom is present in the ion. This digit therefore does not specify the number of like ions in the compound. Examples: Na^+ in NaCl is RGØ.1; $2Na^+$ in Na_2CO_3 is RGØ.1.

7.42 In complex ions, the fourth digit represents the number of like atoms, ions or molecules in the structure of the ion. Examples: O in Na_2SO_4 is U63.4; O in $Al_2(SO_4)_3$ is U63.4; (CN) in $[Fe(CN)_6]^{-4}$ is U44.6.

7.43 In chains of like atoms, the fourth digit represents the number of atoms in the chain. Example: The chain of N atoms in H_2NNH_2 is TG(12).2.

7.44 In intermetallic compounds, the fourth digit represents the number of like atoms in the compound. Example: Cu_2Zn_3 is R7P.2-RV7.3 (R7P = Cu°, RV7 = Zn°).

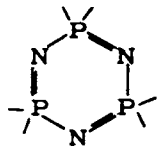
7.45 In free elements, the fourth digit represents the number of atoms in the molecule. Examples: Hg is RC7.1; Cl_2 is T68.2 (RC7 = Hg°, T68 = Cl°).

7.5 Family Q-- classifies ring structures which do not contain carbon. Inorganic compounds with metal coordination rings are coded in Families R--, S--, T-- and U-- (Sec. 7.81). (Chelate structures are coded as open chains.)

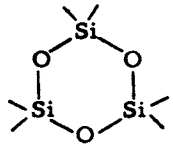
7.51 Multiple ring structures which do not contain carbon in the ring are separated into single rings for coding, common atoms shared by two or more rings being coded as a part of the least number of rings necessary to describe the complete structure (See Sec. 5.61).

7.52 Numbers are assigned to groups in Family Q-- as indicated in the List of Group Numbers. The first digit is the family designation Q, the second digit indicates the number of members in the ring, and the third digit the number of different elements present in the ring. The fourth digit represents the number of such groups in the compound being coded.

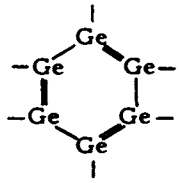
7.53 In addition to numbers in Family Q-- designating the specific ring structure, numbers are also assigned to indicate the occurrence of the individual elements in each ring. The latter numbers are determined in accordance with the principles applicable to Families P--, R--, S--, T-- and U--. Z elements attached to carbon outside of the ring are coded in Family P-- (See Sec. 6.1); central elements which are not attached to carbon are coded in Family R-- or T-- depending upon the electronegativity of the atom (See Sec. 7.65 and 7.75); atoms coordinated to central elements are coded in Family S-- or U-- depending upon the elctronegativity of the central element (See Sec. 7.82). The treatment of an element which is not a Z element and is attached to carbon outside of the Q ring is covered by Sec. 5.98. It should be noted that designation of the elements in Q rings in Families P--, R--, S--, etc. is another example of double coding. Examples:



Q62.1-TJ1.3-U35.3



Q62.1-TP1.3-U63.3



Q61.1-RA(11).6

(Q62 = 6-membered ring (no carbon) containing 2 elements, TJ1 = P^{+5}, U35 = N≡, TP1 = Si^{+4}, U63 = :O or -O-, Q61 = 6-membered ring (no carbon) containing 1 element, RA(11) = Ge chain)

7.6 Family R-- classifies the following "inorganic" groups:

7.61 Free elements other than those in the electronegativity series (Sec. 7.3). Examples: Hg is RC7.1; Al is R15.1.

7.62 Simple cations. Examples: Fe^{+2} is R9P.1; Fe^{+3} is R9Ø.1; Na^{+} is RGØ.1.

7.63 Central atoms in complex cations. Examples: Uranium in UO_2^{+2} is RT2.1 (RT2 = U^{+6}).

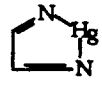
7.631 If a cation consists of two unlike atoms, the more electropositive is considered to be the central atom with the other coordinated to it (See Sec. 7.3).

7.632 In any cation in which two or more atoms are connected to another atom, the latter is designated as the central atom. Example: N in NH_4^{+} is RGI.1 (RGI = N^{-3}).

7.633 In chains of two or more like atoms linked directly together in a cation, these atoms are considered to be the central atoms. Example: Nitrogen in $NH_2NH_3^{+}$ is RG(12).2 (RG(12) = N chain).

7.64 Atoms, other than those included in the electronegativity series (Si, B, Sb, Te, As, P, Se, I, S, C, Br, Cl, N, O, F), which act as central atoms in molecules. Example: Mo in MoO_3 is RG2.1 (RG2 = Mo^{+6}).

7.641 Chains of two or more like elements comprising the central atoms of a molecule, other than Si, B, Sb, Te, As, P, Se, I, S, C, Br, Cl, N, O or F. Free elements are not classified in this way (See Sec. 7.21 and 7.45).

7.65 Elements not listed in the electronegativity series (Sec. 7.3) which are present in ring structures and not attached to ring carbon atoms (See Sec. 5.44 and 7.53). Example: Hg in  is RC5.1 (RC5 = Hg^{+2}).

7.66 Each element in an intermetallic compound (See Sec. 7.22). Example: Cu_2Zn_3 is R7P.2-RV7.3 (R7P = Cu°, RV7 = Zn°).

7.7 Family T-- classifies the following "inorganic" groups:

7.71 Free elements included in the electronegativity series (Si, B, Sb, Te, As, P, Se, I, S, C, Br, Cl, N, O, F).

7.72 Simple anions. Examples: Cl^{-} is T69.1; O^{-2} is TIH.1.

7.73 Central atoms in complex anions. Examples: Sulfur in SO_4^{-2} is TNJ.1; chromium in CrO_4^{-2} is T72.1 (TNJ = S^{+6}, T72 = Cr^{+6}).

7.731 If an anion consists of two unlike atoms, the more electropositive is considered to be the central atom, with the other coordinated to it (See Sec. 7.3). Example: H in OH^{-} is the central atom and is coded as TB6.1

(TB6 = H^{+1}).

7.732 In any anion in which two or more atoms are connected to another atom, the latter is designated as the central atom.

7.733 In chains of two or more like atoms linked directly together in an anion, these atoms are considered to be the central atoms.

7.74 Elements listed in the electronegativity series (Sec. 7.3) which act as central atoms of molecules. Examples: C in CO_2 is T4A.1; Sb in $SbCl_3$ is T$\emptyset$3.1 (T4A = C^{+4}, T$\emptyset$3 = Sb^{+3}).

7.741 If a molecule consists of two unlike atoms, the more electropositive is considered to be the central atom. Example: C in CO is T4C.1 (T4C = C^{+2}).

7.742 In any compound in which two or more atoms are connected to another atom, the latter is designated as the central atom. Examples: N in NH_3 is TGI.1; As in AsH_3 is T1R.1; As in $AsCl_3$ is T1L.1; C in CS_2 is T4I.1 (TGI = N^{-3}, T1R = As^{-3}, T1L = As^{+3}, T4I = C^{-4}).

7.743 Chains of two or more like elements comprising the central atom of a molecule if the elements are included in the electronegativity series (Sec. 7.3). Example: Nitrogen in NH_2NH_2 is TG(12).2 (TG(12) = N chain).

7.75 Elements listed in the electronegativity series (Sec. 7.3) or the more electropositive of two or more such elements which are present in ring structures and are not attached to ring carbon atoms (See Sec. 5.44 and 7.53). Example: Sb in  is T$\emptyset$3.1 (T$\emptyset$3 = Sb^{+3}).

7.8 Families S-- and U-- classify groups coordinated to elements in Family P--, R-- or T--.

7.81 Groups coordinated with central elements in Family P-- are placed in Family S-- if the central element is other than one in the electronegativity series (See Sec. 7.3); they are placed in Family U-- if the central element to which they are coordinated is Si, B, Sb, Te, As, P or Se. (Compounds in which C is attached to N, O, S or halogen are coded as "organic" (See Sec. 2.1, 5.2 and 5.98).) Groups coordinated with elements in Family R-- are classified in Family S--. Groups coordinated with elements in Family T-- are classified in Family U--. Examples:

O in $C_6H_5AsO_3H_2$ is U63.3.

H_2O in $[Cr(H_2O)_6]^{+3}$ is S61.6.

O in $(UO_2)^{+2}$ is S63.2.

O in $(S_2O_7)^{-2}$ is U63.7.

Cl in SCl_4 is UI4.4.

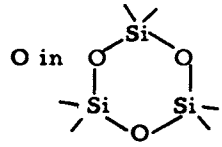
(CN) in $[Fe(CN)_6]^{-4}$ is U44.6.

7.811 A coordinating group (Sec. 1.3) is monodentate when it is attached to the central atom by only one atom of the coordinating group; bidentate when it is attached through two atoms, forming a chelate ring of which the central atom is a member; polydentate when it is attached through three or more atoms, forming a multiple ring system.

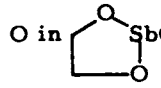
7.812 If a coordinating group is attached to more than one central atom, its mono-, bi- or polydentate character is stated with respect to each single central atom. Example: Ethylenediamine coordinated through two nitrogen atoms to a single metal ion is bidentate, but if the nitrogen atoms of the ethylenediamine molecule are attached to different ions of the metal, the ethylenediamine is monodentate.

7.813 If a coordinating molecule or ion contains two or more different coordinating structures, each of the structures which is attached to the central atom is shown separately. Examples: The coordination character of $H_2NCH_2COO^-$ in $[Co(NH_3)_4(H_2NCH_2COO)]^{+2}$ is coded as S3A.1-S6V.1; of $(CH_3NHCH_2CH_2NH_2)_3$ in $[Cr(CH_3NHCH_2CH_2NH_2)_3]_2^{+3}$ is coded as S3A.3-S3D.3, which indicates three primary and three secondary amine groups coordinated to the chromium (S3A = RNH_2, monodentate; S6V = HCOOH, monodentate; S3D = RR'NH, monodentate). The detailed structure of the organic coordinating molecule or fragment is not indicated in Families S-- and U-- but is coded in the usual manner. In coding $(H_2NCH_2CH_2NH_2)_3$ in $[Cr(H_2NCH_2CH_2NH_2)_3]^{+3}$ as S3B.3, the digits 3B.3 signify that three bidentate primary diamine structures are coordinated with the central element.

7.82 Elements present in ring structures and not attached to ring carbon atoms, but which, because of their attachment to more electropositive elements, cannot be coded in Family R-- or T--, are coded in Family S-- or U-- (cf. Sec. 7.65 and 7.75). N, O or S attached to a Z element and carbon are coded in Family S-- or U-- depending on the nature of the Z element as described in Sec. 5.98. Examples:

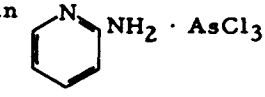


is U63.3 (U63 = :O or -O-).



is U63.3 (U63 = :O or -O-).

7.9 Family V-- classifies solvate molecules which are associated but not chemically coordinated with inorganic or organic compounds. Examples: The $2H_2O$ in $[Cr(H_2O)_4Cl_2]Cl\cdot 2H_2O$ is coded as V61.2; the $4CH_3OH$ in $CaCl_2\cdot 4CH_3OH$ is coded as V6A.4 (V61 = H_2O; V6A = ROH, monodentate). In the case of fractions the next higher number is used. Example: $1\text{-}1/2H_2O$ is coded as V61.2.

7.91 Molecular addition compounds containing molecules not included in the List of Coordinate and Solvate Groups (pp. 67-71) are coded by numbers representing all constituents of the molecule. Example: $AsCl_3$ in  is T1L.1-UI4.3 (T1L = As^{+3}, UI4 = -Cl).

LIST OF GROUP NUMBERS

DIVISION I - ORGANIC GROUPS

FAMILIES 0-- to ø--

(CH)NOSX

Difluorosulfonamides	HSO_2NF_2	021
Dichlorosulfonamides	HSO_2NCl_2	022
Dibromosulfonamides	HSO_2NBr_2	023
Diiodosulfonamides	HSO_2NI_2	024
Dihalosulfonamides (unspecified)	HSO_2NX_2	029
Chlorofluorosulfonamides	HSO_2NFCl	031
Bromofluorosulfonamides	HSO_2NFBr	032
Fluoroiodosulfonamides	HSO_2NFI	033
Bromochlorosulfonamides	HSO_2NClBr	034
Chloroiodosulfonamides	HSO_2NClI	035
Bromoiodosulfonamides	HSO_2NBrI	036
Halohalosulfonamides (unspecified)	HSO_2NXX'	039
Fluorosulfonamides	HSO_2NHF	041
Chlorosulfonamides	HSO_2NHCl	042
Bromosulfonamides	HSO_2NHBr	043
Iodosulfonamides	HSO_2NHI	044
Halosulfonamides (unspecified)	HSO_2NHX	049
Sulfamyl fluorides	H_2NSO_2F	051
Sulfamyl chlorides	H_2NSO_2Cl	052
Sulfamyl bromides	H_2NSO_2Br	053
Sulfamyl iodides	H_2NSO_2I	054
Sulfamyl halides (unspecified)	H_2NSO_2X	059

(CH)NOS - NONCYCLIC GROUPS*

Dicarboxamidosulfides	HC(:O)NHSNHC(:O)H	120
Thio(or dithio)diacylureas	HC(:O)NHC(:S)NHC(:O)H, HC(:S)NHC(:O)NHC(:O)H, HC(:S)NHC(:S)NHC(:O)H or HC(:S)NHC(:O)NHC(:S)H (includes tautomers)	123
Thioacylureas	$HC(:O)NHC(:S)NH_2$ or $HC(:S)NHC(:O)NH_2$ (includes tautomers)	124
Thiocarbamates	$NH_2C(:S)OH$ or $NH_2C(:O)SH$ (includes tautomers)	125
Azosulfonates	$HN:NSO_3H$	130
Hydrazinesulfonates	H_2NNHSO_3H	131
Sulfonylhydrazines	H_2NNHSO_2H	133
Hydrazinesulfinates	$H_2NNHS(:O)OH$	135
Sulfinylhydrazines	$H_2NN:S:O$	138
Sulfinylamines	HN:S:O	139

* This includes fragments of heterocyclic rings containing a part of the group outside of the ring.

CNOS(Z) RINGS

CNOSZ

CNOS

(CH)NOX

(CH)NSX

Chlorofluorothioamides	HC(:S)NFCl	431
Bromofluorothioamides	HC(:S)NFBr	432
Fluoroiodothioamides	HC(:S)NFI	433
Bromochlorothioamides	HC(:S)NClBr	434
Chloroiodothioamides	HC(:S)NClI	435
Bromoiodothioamides	HC(:S)NBrI	436
Halohalothioamides (unspecified)	HC(:S)NXX'	439
Fluorothioamides	HC(:S)NHF or HC(:NF)SH	441
Chlorothioamides	HC(:S)NHCl or HC(:NCl)SH	442
Bromothioamides	HC(:S)NHBr or HC(:NBr)SH	443
Iodothioamides	HC(:S)NHI or HC(:NI)SH	444
Halothioamides (unspecified)	HC(:S)NHX or HC(:NX)SH	449

(CH)OSX

Fluorosulfonates	FSO_2OH	511
Chlorosulfonates	$ClSO_2OH$	512
Bromosulfonates	$BrSO_2OH$	513
Iodosulfonates	ISO_2OH	514
Halosulfonates (unspecified)	XSO_2OH	519
Sulfonyl fluorides	HSO_2F	521
Sulfonyl chlorides	HSO_2Cl	522
Sulfonyl bromides	HSO_2Br	523
Sulfonyl iodides	HSO_2I	524
Sulfonyl halides (unspecified)	HSO_2X	529
Sulfinyl fluorides	HS(:O)F	531
Sulfinyl chlorides	HS(:O)Cl	532
Sulfinyl bromides	HS(:O)Br	533
Sulfinyl iodides	HS(:O)I	534
Sulfinyl halides (unspecified)	HS(:O)X	539

(CH)NO - NONCYCLIC GROUPS*

Guanylureas	$H_2NC(:NH)NHC(:O)NH_2$	610
Carbohydrazones	$R:NNHC(:O)NHNH_2$	615
Carbohydrazides	$H_2NNHC(:O)NHNH_2$	616
Semicarbazones	$R:NNHC(:O)NH_2$	620
Semicarbazides	$H_2NNHC(:O)NH_2$	621
Diacylureas	HC(:O)NHC(:O)NHC(:O)H (includes tautomers)	623
Acylureas	$HC(:O)NHC(:O)NH_2$ (includes tautomers)	624
Ureas or pseudoureas	$H_2NC(:O)NH_2$ or $H_2NC(:NH)OH$	625
Hydrazides	$HC(:O)NHNH_2$	629
Carbamic acid esters	R'-NC(:O)OR	630
	R'R''NC(:O)OR	632
	R'HNC(:O)OR	634
	$H_2NC(:O)OR$	637
Carbamic acids	$H_2NC(:O)OH$	639

* This includes fragments of heterocyclic rings containing a part of the group outside of the ring.

CNO(Z) RINGS

CNOZ

9- or more-membered rings
- Complete saturation 70K
- Unsaturation other than maximum . 70N
- Maximum unsaturation 70R

8-membered rings
- Complete saturation 712
- Unsaturation other than maximum . 715
- Maximum unsaturation 719

7-membered rings
- Complete saturation 71K
- Unsaturation other than maximum . 71N
- Maximum unsaturation 71R

6-membered rings
- Complete saturation 722
- Unsaturation other than maximum . 725
- Maximum unsaturation 729

5-membered rings
- Complete saturation 72K
- Unsaturation other than maximum . 72N
- Maximum unsaturation 72R

4-membered rings
- Complete saturation 732
- Unsaturation other than maximum . 735
- Maximum unsaturation 739

CNO

9- or more-membered rings
- Complete saturation 752
- Unsaturation other than maximum . 755
- Maximum unsaturation 759

8-membered rings
- Complete saturation 762
- Unsaturation other than maximum . 765
- Maximum unsaturation 769

7-membered rings

CN_xO_{6-x}
- Complete saturation 772
- Unsaturation other than maximum . 775
- Maximum unsaturation 779

$C_2N_xO_{5-x}$
- Complete saturation 77K
- Unsaturation other than maximum . 77N
- Maximum unsaturation 77R

$C_3N_xO_{4-x}$
- Complete saturation 782
- Unsaturation other than maximum . 785
- Maximum unsaturation 789

$C_4N_xO_{3-x}$
- Complete saturation 78K
- Unsaturation other than maximum . 78N
- Maximum unsaturation 78R

C_5NO
- Complete saturation 792
- Unsaturation other than maximum . 795
- Maximum unsaturation 799

6-membered rings

CNO_4
- Complete saturation 7A2
- Unsaturation other than maximum . 7A5
- Maximum unsaturation 7A9

CN_2O_3
- Complete saturation 7AK
- Unsaturation other than maximum . 7AN
- Maximum unsaturation 7AR

CN_3O_2
- Complete saturation 7B2
- Unsaturation other than maximum . 7B5
- Maximum unsaturation 7B9

CN_4O
- Complete saturation 7C2
- Unsaturation other than maximum . 7C5
- Maximum unsaturation 7C9

C_2NO_3
- Complete saturation 7D2
- Unsaturation other than maximum . 7D5
- Maximum unsaturation 7D9

$C_2N_2O_2$
- Complete saturation 7E2
- Unsaturation other than maximum . 7E5
- Maximum unsaturation 7E9

C_2N_3O
- Complete saturation 7F2
- Unsaturation other than maximum . 7F5
- Maximum unsaturation 7F9

C_3NO_2
- Complete saturation 7G2
- Unsaturation other than maximum . 7G5
- Maximum unsaturation 7G9

C_3N_2O
- Complete saturation 7H2
- Unsaturation other than maximum . 7H5
- Maximum unsaturation 7H9

C_4NO
- Complete saturation 7I2
- Unsaturation other than maximum . 7I5
- Maximum unsaturation 7I9

5-membered rings

CNO_3
- Complete saturation 7J2
- Unsaturation other than maximum . 7J5
- Maximum unsaturation 7J9

CN_2O_2
- Complete saturation 7K2
- Unsaturation other than maximum . 7K5
- Maximum unsaturation 7K9

CN_3O
- Complete saturation 7L2
- Unsaturation other than maximum . 7L5
- Maximum unsaturation 7L9

C_2NO_2
- Complete saturation 7M2
- Unsaturation other than maximum . 7M5
- Maximum unsaturation 7M9

C_2N_2O
- Complete saturation 7N2
- Unsaturation other than maximum . 7N5
- Maximum unsaturation 7N9

C_3NO
- Complete saturation 7Ø2
- Unsaturation other than maximum . 7Ø5
- Maximum unsaturation 7Ø9

4-membered rings

CNO_2
- Complete saturation 7S2
- Unsaturation other than maximum . 7S5
- Maximum unsaturation 7S9

CN_2O
- Complete saturation 7T2
- Unsaturation other than maximum . 7T5
- Maximum unsaturation 7T9

C_2NO
- Complete saturation 7V2
- Unsaturation other than maximum . 7V5
- Maximum unsaturation 7V9

3-membered rings

CNO
- Saturated 7W2
- Unsaturated 7W9

(CH)NS - NONCYCLIC GROUPS*

Bis(thiocarbamyl) polysulfides	$H_2NC(:S)S_xC(:S)NH_2$ (x > 1)	805
Bis(thiocarbamyl) sulfides	$H_2NC(:S)SC(:S)NH_2$	808
Thiocarbohydrazones	$R:NNHC(:S)NHNH_2$	815
Thiocarbohydrazides	$H_2NNHC(:S)NHNH_2$	816
Thiosemicarbazones	$R:NNHC(:S)NH_2$	820
Thiosemicarbazides	$H_2NNHC(:S)NH_2$	821
Trithiodiacylureas	HC(:S)NHC(:S)NHC(:S)H (includes tautomers)	823
Dithioacylureas	HC(:S)NHC(:S)NH_2 (includes tautomers)	824
Thioureas or thiopseudoureas	$H_2NC(:S)NH_2$ or $H_2NC(:NH)SH$	825
Thiohydrazides	$HC(:S)NHNH_2$	829
Dithiocarbamates	$H_2NC(:S)SH$ or (HN:)C(SH)SH	830
Dithioimides	HC(:S)NHC(:S)H	843
Thioimido esters	HC(SR)(:NH)	849
Thioamides	HC(:S)N-R	850
	HC(:S)NRR'	851
	HC(:S)NHR or HC(SH)(:NR)	852
	HC(:S)NH_2 or HC(SH)(:NH)	853
Thiocyanates	HSCN	861
Isothiocyanates	HNCS	862
Diaminosulfides	H_2NSNH_2	868
Sulfimes	R:NSH	875
Hydrosulfamines or sulfenamides	$HSNH_2$	877
Sulfilimines	$H_2S:NH$	880

* This includes fragments of heterocyclic rings containing a part of the group outside of the ring.

CNO(Z) (CH)NS
CNS(Z) (CH)OS
COS(Z) (CH)NX (CH)OX

CNS(Z) RINGS

CNSZ

9- or more-membered rings
- Complete saturation 90K
- Unsaturation other than maximum . 90N
- Maximum unsaturation 90R

8-membered rings
- Complete saturation 912
- Unsaturation other than maximum . 915
- Maximum unsaturation 919

7-membered rings
- Complete saturation 91K
- Unsaturation other than maximum . 91N
- Maximum unsaturation. 91R

6-membered rings
- Complete saturation 922
- Unsaturation other than maximum . 925
- Maximum unsaturation 929

5-membered rings
- Complete saturation 92K
- Unsaturation other than maximum . 92N
- Maximum unsaturation 92R

4-membered rings
- Complete saturation 932
- Unsaturation other than maximum . 935
- Maximum unsaturation 939

CNS

9- or more-membered rings
- Complete saturation 952
- Unsaturation other than maximum . 955
- Maximum unsaturation 959

8-membered rings
- Complete saturation 962
- Unsaturation other than maximum . 965
- Maximum unsaturation 969

7-membered rings

CN_xS_{6-x}
- Complete saturation 972
- Unsaturation other than maximum . 975
- Maximum unsaturation 979

$C_2N_xS_{5-x}$
- Complete saturation 97K
- Unsaturation other than maximum . 97N
- Maximum unsaturation 97R

$C_3N_xS_{4-x}$
- Complete saturation 982
- Unsaturation other than maximum . 985
- Maximum unsaturation 989

$C_4N_xS_{3-x}$
- Complete saturation 98K
- Unsaturation other than maximum . 98N
- Maximum unsaturation 98R

C_5NS
- Complete saturation 992
- Unsaturation other than maximum . 995
- Maximum unsaturation 999

6-membered rings

CNS_4
- Complete saturation 9A2
- Unsaturation other than maximum . 9A5
- Maximum unsaturation 9A9

CN_2S_3
- Complete saturation 9AK
- Unsaturation other than maximum . 9AN
- Maximum unsaturation 9AR

CN_3S_2
- Complete saturation 9B2
- Unsaturation other than maximum . 9B5
- Maximum unsaturattion 9B9

CN_4S
- Complete saturation 9C2
- Unsaturation other than maximum . 9C5
- Maximum unsaturation 9C9

C_2NS_3
- Complete saturation 9D2
- Unsaturation other than maximum . 9D5
- Maximum unsaturation 9D9

$C_2N_2S_2$
- Complete saturation 9E2
- Unsaturation other than maximum . 9E5
- Maximum unsaturation 9E9

C_2N_3S
- Complete saturation 9F2
- Unsaturation other than maximum . 9F5
- Maximum unsaturation 9F9

C_3NS_2
- Complete saturation 9G2
- Unsaturation other than maximum . 9G5
- Maximum unsaturation 9G9

C_3N_2S
- Complete saturation 9H2
- Unsaturation other than maximum . 9H5
- Maximum unsaturation 9H9

C_4NS
- Complete saturation 9I2
- Unsaturation other than maximum . 9I5
- Maximum unsaturation 9I9

5-membered rings

CNS_3
- Complete saturation 9J2
- Unsaturation other than maximum . 9J5
- Maximum unsaturation 9J9

CN_2S_2
- Complete saturation 9K2
- Unsaturation other than maximum . 9K5
- Maximum unsaturation 9K9

CN_3S
- Complete saturation 9L2
- Unsaturation other than maximum . 9L5
- Maximum unsaturation 9L9

C_2NS_2
- Complete saturation 9M2
- Unsaturation other than maximum . 9M5
- Maximum unsaturation 9M9

C_2N_2S
- Complete saturation 9N2
- Unsaturation other than maximum . 9N5
- Maximum unsaturation 9N9

C_3NS
- Complete saturation 9Ø2
- Unsaturation other than maximum . 9Ø5
- Maximum unsaturation 9Ø9

4-membered rings

CNS_2
- Complete saturation 9S2
- Unsaturation other than maximum . 9S5
- Maximum unsaturation 9S9

CN_2S
- Complete saturation 9T2
- Unsaturation other than maximum . 9T5
- Maximum unsaturation 9T9

C_2NS
- Complete saturation 9V2
- Unsaturation other than maximum . 9V5
- Maximum unsaturation 9V9

3-membered rings
- Saturated 9W2
- Unsaturated 9W9

(CH)OS - NONCYCLIC GROUPS*

Dithiocarbonates	HOC(:S)SH or HSC(:O)SH	A15
Thiocarbonates	HOC(:S)OH or HSC(:O)OH	A18
Carbothioates	HC(:O)SH or HC(:S)OH	A20
Sultones	$RS(:O)_2O$	A36
Sulfonates	HSO_3H	A42
Thiosulfonates	$HS_nO_{4-n}H$	A43
Sulfinates	HS(:O)OH	A47
Thiosulfinates	HS(:O)SH or HS(:S)OH	A48
Hexathionates	RHS_6O_6	A51
Pentathionates	RHS_5O_6	A52
Tetrathionates	RHS_4O_6	A53
Trithionates	RHS_3O_6	A54
Dithionates	RHS_2O_6	A55
Dithionites	RHS_2O_4	A56
Thiosulfates	RHS_2O_3	A61
Sulfates	$RHSO_4$	A64
Sulfites	$RHSO_3$	A69
Sulfones	$RR'SO_2$	A70
Sulfoxides	RR'SO	A76
Sulfenates	HSOH	A80

* This includes fragments of heterocyclic rings containing a part of the group outside of the ring.

COS(Z) RINGS

COSZ

9- or more-membered rings
- Complete saturation B0K
- Unsaturation other than maximum . B0N
- Maximum unsaturation B0R

8-membered rings
- Complete saturation B12
- Unsaturation other than maximum . B15
- Maximum unsaturation B19

7-membered rings
- Complete saturation B1K
- Unsaturation other than maximum . B1N
- Maximum unsaturation B1R

6-membered rings
- Complete saturation B22
- Unsaturation other than maximum . B25
- Maximum unsaturation B29

5-membered rings
- Complete saturation B2K
- Unsaturation other than maximum . B2N
- Maximum unsaturation B2R

4-membered rings
- Complete saturation B32
- Unsaturation other than maximum . B35
- Maximum unsaturation B39

COS

9- or more-membered rings
- Complete saturation B52
- Unsaturation other than maximum . B55
- Maximum unsaturation B59

8-membered rings
- Complete saturation B62
- Unsaturation other than maximum . B65
- Maximum unsaturation B69

7-membered rings

CO_xS_{6-x}
- Complete saturation B72
- Unsaturation other than maximum . B75
- Maximum unsaturation B79

$C_2O_xS_{5-x}$
- Complete saturation B7K
- Unsaturation other than maximum . B7N
- Maximum unsaturation B7R

$C_3O_xS_{4-x}$
- Complete saturation B82
- Unsaturation other than maximum . B85
- Maximum unsaturation B89

$C_4O_xS_{3-x}$
- Complete saturation B8K
- Unsaturation other than maximum . B8N
- Maximum unsaturation B8R

C_5OS
- Complete saturation B92
- Unsaturation other than maximum . B95
- Maximum unsaturation B99

6-membered rings

COS_4
- Complete saturation BA2
- Unsaturation other than maximum . BA5
- Maximum unsaturation BA9

CO_2S_3
- Complete saturation . . . . . BAK
- Unsaturation other than maximum . BAN
- Maximum unsaturation . . . . . BAR

CO_3S_2
- Complete saturation BB2
- Unsaturation other than maximum . BB5
- Maximum unsaturation BB9

CO_4S
- Complete saturation BC2
- Unsaturation other than maximum . BC5
- Maximum unsaturation BC9

C_2OS_3
- Complete saturation BD2
- Unsaturation other than maximum . BD5
- Maximum unsaturation BD9

$C_2O_2S_2$
- Complete saturation BE2
- Unsaturation other than maximum . BE5
- Maximum unsaturation BE9

C_2O_3S
- Complete saturation BF2
- Unsaturation other than maximum . BF5
- Maximum unsaturation BF9

C_3OS_2
- Complete saturation BG2
- Unsaturation other than maximum . BG5
- Maximum unsaturation BG9

C_3O_2S
- Complete saturation BH2
- Unsaturation other than maximum . BH5
- Maximum unsaturation BH9

C_4OS
- Complete saturation BI2
- Unsaturation other than maximum . BI5
- Maximum unsaturation BI9

5-membered rings

COS_3
- Complete saturation BJ2
- Unsaturation other than maximum . BJ5
- Maximum unsaturation BJ9

CO_2S_2
- Complete saturation BK2
- Unsaturation other than maximum . BK5
- Maximum unsaturation BK9

CO_3S
- Complete saturation BL2
- Unsaturation other than maximum . BL5
- Maximum unsaturation BL9

C_2OS_2
- Complete saturation BM2
- Unsaturation other than maximum . BM5
- Maximum unsaturation BM9

C_2O_2S
- Complete saturation BN2
- Unsaturation other than maximum . BN5
- Maximum unsaturation BN9

C_3OS
- Complete saturation BØ2
- Unsaturation other than maximum . BØ5
- Maximum unsaturation BØ9

CO_2S
- Complete saturation BT2
- Unsaturation other than maximum . BT5
- Maximum unsaturation BT9

C_2OS
- Complete saturation BV2
- Unsaturation other than maximum . BV5
- Maximum unsaturation BV9

4-membered rings

COS_2
- Complete saturation BS2
- Unsaturation other than maximum . BS5
- Maximum unsaturation BS9

3-membered rings

COS
- Saturated BW2
- Unsaturated BW9

(CH)NX

Haloamidines	$HC(NH_2)(:NX)$	C15
Difluoroamines	HNF_2	C21
Dichloroamines	$HNCl_2$	C22
Dibromoamines	$HNBr_2$	C23
Diiodoamines	HNI_2	C24
Dihaloamines (unspecified)	HNX_2	C29
Chlorofluoroamines	HNFCl	C31
Bromofluoroamines	HNFBr	C32
Fluoroiodoamines	HNFI	C33
Bromochloroamines	HNClBr	C34
Chloroiodoamines	HNClI	C35
Bromoiodoamines	HNBrI	C36
Halohaloamines (unspecified)	HNXX'	C39
Fluoroimines	R:NF	C41
Chloroimines	R:NCl	C42
Bromoimines	R:NBr	C43
Iodoimines	R:NI	C44
Haloimines (unspecified)	R:NX	C49
Fluoroamines	H_2NF	C51
Chloroamines	H_2NCl	C52
Bromoamines	H_2NBr	C53
Iodoamines	H_2NI	C54
Haloamines (unspecified)	H_2NX	C59

(CH)OX

Haloformate	XC(:O)OH	D15
Acyl fluorides	HC(:O)F	D21
Acyl chlorides	HC(:O)Cl	D22
Acyl bromides	HC(:O)Br	D23
Acyl iodides	HC(:O)I	D24
Acyl halides (unspecified)	HC(:O)X	D29

Iodoso compounds	HIO	D40
Iodoxy compounds	HIO_2	D41
Halo-oxygen acid esters	RXO_n	D49

(CH)SX

Thioacyl halides	HC(:S)X	E29
Sulfenyl fluorides	HSF	E31
Sulfenyl chlorides	HSCl	E32
Sulfenyl bromides	HSBr	E33
Sulfenyl iodides	HSI	E34
Sulfenyl halides (unspecified)	HSX	E39

(CH)N - NONCYCLIC GROUPS*

Biguanides	$H_2NC(:NH)NHC(:NH)NH_2$	F10
Guanidines	$H_2NC(:NH)NH_2$	F15
Amidines	$HC(:NH)NH_2$	F17
Triazenes	$HN:NNH_2$	F20
Azides	HN_3	F23
Azo or diazo compounds	HN:NH	F25
Diazonium compounds	$(HN:N)^+$	F28
Hydrazones	$R:NNH_2$	F30
Hydrazines	H_2NNH_2	F35
Quaternary ammonium compounds	$RR':N^+$ (: may be resonating double bond)	F41
	$RR'R''-N^+$ or $RR'-N^+$	F43
	$RR'R'':N^+$ or $RR'R''R'''N^+$	F46
	$>N^{+}<$ or $[N]^+$ (This group cannot be attached to H and must be attached to at least one element other than C)	F47
Imines	R:NH	F4T
Amines, tertiary	R:N (: may be resonating double bond)	F50
	R-NR' or R-N	F51
	$RR'R''N$	
	R,R',R'' are heterocyclic	F52
	R,R',R'' are aromatic carbocyclic	F53
	R,R',R'' are alicyclic or aliphatic	F54
	R,R',R'' are heterocyclic and aromatic carbocyclic	F55
	R,R',R'' are heterocyclic and alicyclic or aliphatic	F56
	R,R',R'' are aromatic carbocyclic and alicyclic or aliphatic	F57
	R,R',R'' are heterocyclic, aromatic carbocyclic and alicyclic or aliphatic	F58

* This includes fragments of heterocyclic rings containing a part of the group outside of the ring.

secondary . . . . . R-NH F5A
RR'NH
R and R' are heterocyclic F5B
R and R' are aromatic carbocyclic . . . F5C
R and R' are alicyclic or aliphatic . . . F5D
R and R' are heterocyclic and aromatic carbocyclic F5E
R and R' are heterocyclic and alicyclic or aliphatic F5F
R and R' are aromatic carbocyclic and alicyclic or aliphatic F5G

primary . . . . . RNH_2
R is heterocyclic F5K
R is aromatic carbocyclic F5L
R is alicyclic or aliphatic F5M

tertiary, secondary or primary. . . . RNH_2
R is unspecified F5R

Cyanamides . . . . . H_2NCN F70
Cyanides or nitriles . . . . . HCN F75
Isocyanides . . . . . HNC F78

CN(Z) RINGS

CNZ

9- or more-membered rings
Complete saturation G0K
Unsaturation other than maximum . G0N
Maximum unsaturation G0R

8-membered rings
Complete saturation G12
Unsaturation other than maximum . G15
Maximum unsaturation G19

7-membered rings
Complete saturation G1K
Unsaturation other than maximum . G1N
Maximum unsaturation G1R

6-membered rings
Complete saturation G22
Unsaturation other than maximum . G25
Maximum unsaturation G29

5-membered rings
Complete saturation G2K
Unsaturation other than maximum . G2N
Maximum unsaturation G2R

4-membered rings
Complete saturation G32
Unsaturation other than maximum . G35
Maximum unsaturation G39

3-membered rings
Saturated G3K
Unsaturated G3R

CN

10- or more-membered rings
Complete saturation G42
Unsaturation other than maximum . G45
Maximum unsaturation G49

9-membered rings
Complete saturation G52
Unsaturation other than maximum . G55
Maximum unsaturation G59

8-membered rings
Complete saturation G62
Unsaturation other than maximum . G65
Maximum unsaturation G69

7-membered rings
CN_6
Complete saturation G72
Unsaturation other than maximum . G75
Maximum unsaturation G79
C_2N_5
Complete saturation. G7K
Unsaturation other than maximum . G7N
Maximum unsaturation G7R
C_3N_4
Complete saturation G82
Unsaturation other than maximum . G85
Maximum unsaturation G89
C_4N_3
Complete saturation G8K
Unsaturation other than maximum . G8N
Maximum unsaturation G8R

C_5N_2
- Complete saturation G92
- Unsaturation other than maximum . G95
- Maximum unsaturation G99

C_6N
- Complete saturation G9K
- Unsaturation other than maximum . G9N
- Maximum unsaturation G9R

6-membered rings

CN_5
- Complete saturation GA2
- Unsaturation other than maximum . GA5
- Maximum unsaturation GA9

C_2N_4
- Complete saturation GB2
- Unsaturation other than maximum . GB5
- Maximum unsaturation GB9

C_3N_3
- Complete saturation GD2
- Unsaturation other than maximum . GD5
- Maximum unsaturation GD9

C_4N_2 (1,2-diazine)
- Complete saturation GF2
- One unsaturation GF3
- Two unsaturations GF4
- Maximum unsaturation GF9

C_4N_2 (1,3-diazine)
- Complete saturation . . . . . GFB
- One unsaturation . . . . . GFC
- Two unsaturations . . . . . GFD
- Maximum unsaturation . . . . . GFI

C_4N_2 (1,4-diazine)
- Complete saturation . . . . . GFK
- One unsaturation . . . . . GFL
- Two unsaturations . . . . . GFM
- Maximum unsaturation . . . . . GFR

C_5N
- Complete saturation* GG2
- One unsaturation* GG3
- Two unsaturations* GG4
- Maximum unsaturation* GG9

* Fused to another ring structure

C_5N
- Complete saturation GH2
- One unsaturation GH3
- Two unsaturations GH4
- Maximum unsaturation GH9

5-membered rings

CN_4
- Complete saturation GJ2
- Unsaturation other than maximum . GJ5
- Maximum unsaturation GJ9

C_2N_3
- Complete saturation GL2
- Unsaturation other than maximum . GL5
- Maximum unsaturation GL9

C_3N_2
- Complete saturation GN2
- Unsaturation other than maximum . GN5
- Maximum unsaturation GN9

C_4N
- Complete saturation GP2
- Unsaturation other than maximum . GP5
- Maximum unsaturation GP9

4-membered rings

CN_3
- Complete saturation GS2
- Unsaturation other than maximum . GS5
- Maximum unsaturation GS9

C_2N_2
- Complete saturation GT2
- Unsaturation other than maximum . GT5
- Maximum unsaturation GT9

C_3N
- Complete saturation GV2
- Unsaturation other than maximum . GV5
- Maximum unsaturation GV9

3-membered rings

CN_2
- Saturated GW2
- Unsaturated GW9

C_2N
- Saturated GX2
- Unsaturated GX9

(CH)O - NONCYCLIC GROUPS**

Peroxides	ROO	H10
	HOOH	H11
Orthocarbonates	$C(OH)_4$	H13
Carbonates	HOC(:O)OH	H15
Acid anhydrides	HC(:O)OC(:O)H	H23
Orthocarboxylates	$HC(OH)_3$	H25
Lactones	RC(:O)O	H26

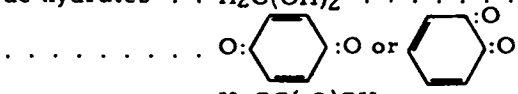
** This includes fragments of heterocyclic rings containing a part of the group outside of the ring.

Carboxylic acid esters . . . . . RC(:O)OR'
- R and R' are heterocyclic H30
- R and R' are aromatic carbocyclic . . . H31
- R and R' are alicyclic or aliphatic (R may be H) H32
- R is heterocyclic
  - and R' is aromatic carbocyclic H33
  - and R' is alicyclic or aliphatic H34
- R is aromatic carbocyclic
  - and R' is heterocyclic. H35
  - and R' is alicyclic or aliphatic H36
- R is alicyclic or aliphatic (R may be H)
  - and R' is heterocyclic. H37
  - and R' is aromatic carbocyclic H38
- R or R' is unspecified (R may be H). . . H39

Carboxylic acids . . . . . RC(:O)OH
- R is heterocyclic H40
- R is aromatic carbocyclic H41
- R is alicyclic or aliphatic (R may be H). H42
- R is unspecified H48

Acetals . . . . . $\underline{ROCH_2O}$ H4J

Acetals, hemiacetals or aldehyde hydrates . . $\underline{H_2C(OH)_2}$ H4M

Quinones . . . . .  H50

Ketones . . . . . $\underline{H_2CC(:O)CH_2}$ H51

RC(:O)R'
- R and R' are heterocyclic H52
- R and R' are aromatic carbocyclic . . . H53
- R and R' are alicyclic or aliphatic . . . H54
- R and R' are heterocyclic and aromatic carbocyclic. H55
- R and R' are heterocyclic and alicyclic or aliphatic H56
- R and R' are aromatic carbocyclic and alicyclic or aliphatic H57
- R or R' is unspecified H59

Aldehydes . . . . . RC(:O)H
- R is heterocyclic H5B
- R is aromatic carbocyclic H5C
- R is alicyclic or aliphatic (R may be H). H5D
- R is unspecified H5G

Nonketonic carbonyl groups . . . . . -C(:O)- H5I

Ethers . . . . . $\underline{R\text{-}O}$ H61

ROR'
- R and R' are heterocyclic H62
- R and R' are aromatic carbocyclic . . . H63
- R and R' are alicyclic or aliphatic . . . H64
- R and R' are heterocyclic and aromatic carbocyclic H65
- R and R' are heterocyclic and alicyclic or aliphatic H66
- R and R' are aromatic carbocyclic and alicyclic or aliphatic H67
- R or R' is unspecified H69

Phenols . . . . . ROH
- R is aromatic heterocyclic H72
- R is aromatic polycarbocyclic H73
- R is aromatic monocarbocyclic H74

Alcohols, tertiary	$\underline{R}\text{-}\underline{C}(OH)R'$, $\overline{R\text{-}C}OH$ or $\underline{R}:\underline{C}OH$	H81
	$RR'R''COH$	
	R,R',R'' are heterocyclic	H82
	R,R',R'' are aromatic carbocyclic	H83
	R,R',R'' are alicyclic or aliphatic	H84
	R,R',R'' are heterocyclic and aromatic carbocyclic	H85
	R,R',R'' are heterocyclic and alicyclic or aliphatic	H86
	R, R',R'' are aromatic carbocyclic and alicyclic or aliphatic	H87
	R,R',R'' are heterocyclic, aromatic carbocyclic and alicyclic or aliphatic	H88
Tertiary carbinol groups	$\geq COH$ (This group cannot be attached to H and must be attached to at least one element other than C)	H89
Alcohols, secondary	$\underline{R}\text{-}\underline{C}HOH$	H8A
	$RR'CHOH$	
	R and R' are heterocyclic	H8B
	R and R' are aromatic carbocyclic	H8C
	R and R' are alicyclic or aliphatic	H8D
	R and R' are heterocyclic and aromatic carbocyclic	H8E
	R and R' are heterocyclic and alicyclic or aliphatic	H8F
	R and R' are aromatic carbocyclic and alicyclic or aliphatic	H8G
Secondary carbinol groups	$>CHOH$ (This group cannot be attached to H and must be attached to at least one element other than C)	H8I
Alcohols, primary	RCH_2OH	
	R is heterocyclic	H8K
	R is aromatic carbocyclic	H8L
	R is alicyclic or aliphatic (R may be H)	H8M
Primary carbinol groups	$-CH_2OH$ (This group cannot be attached to H and must be attached to an element other than C)	H8R
Alcohols or phenols	ROH (R is unspecified)	H8Z
Oxonium compounds	RH_2O^+, $\underline{R}\text{-}\underline{O}H^+$, $\overline{R\text{-}O}^+$ or $\underline{R}:\underline{O}^+$ (: may be resonating double bond)	H90

CO(Z) RINGS

COZ

9- or more-membered rings
- Complete saturation I0K
- Unsaturation other than maximum . I0N
- Maximum unsaturation I0R

8-membered rings
- Complete saturation I12
- Unsaturation other than maximum . I15
- Maximum unsaturation I19

7-membered rings
- Complete saturation I1K
- Unsaturation other than maximum . I1N
- Maximum unsaturation I1R

6-membered rings
- Complete saturation I22
- Unsaturation other than maximum . I25
- Maximum unsaturation I29

5-membered rings
- Complete saturation I2K
- Unsaturation other than maximum . I2N
- Maximum unsaturation I2R

4-membered rings
- Complete saturation I32
- Unsaturation other than maximum . I35
- Maximum unsaturation I39

3-membered rings
- Saturated I3K
- Unsaturated I3R

CO

10- or more-membered rings
- Complete saturation I42
- Unsaturation other than maximum . I45
- Maximum unsaturation I49

9-membered rings
- Complete saturation I52
- Unsaturation other than maximum . I55
- Maximum unsaturation I59

8-membered rings
- Complete saturation I62
- Unsaturation other than maximum . I65
- Maximum unsaturation. I69

7-membered rings

CO_6
- Complete saturation I72
- Unsaturation other than maximum . I75
- Maximum unsaturation I79

C_2O_5
- Complete saturation I7K
- Unsaturation other than maximum . I7N
- Maximum unsaturation I7R

C_3O_4
- Complete saturation I82
- Unsaturation other than maximum . I85
- Maximum unsaturation I89

C_4O_3
- Complete saturation I8K
- Unsaturation other than maximum . I8N
- Maximum unsaturation I8R

C_5O_2
- Complete saturation I92
- Unsaturation other than maximum . I95
- Maximum unsaturation I99

C_6O
- Complete saturation I9K
- Unsaturation other than maximum . I9N
- Maximum unsaturation I9R

6-membered rings

CO_5
- Complete saturation IA2
- Unsaturation other than maximum . IA5
- Maximum unsaturation IA9

C_2O_4
- Complete saturation IB2
- Unsaturation other than maximum . IB5
- Maximum unsaturation IB9

C_3O_3
- Complete saturation ID2
- Unsaturation other than maximum . ID5
- Maximum unsaturation ID9

C_4O_2
- Complete saturation IF2
- Unsaturation other than maximum . IF5
- Maximum unsaturation IF9

C_5O
- Complete saturation IH2
- Unsaturation other than maximum . IH5
- Maximum unsaturation IH9

5-membered rings

CO_4
- Complete saturation IJ2
- Unsaturation other than maximum . IJ5
- Maximum unsaturation IJ9

C_2O_3
- Complete saturation IL2
- Unsaturation other than maximum . IL5
- Maximum unsaturation IL9

C_3O_2
- Complete saturation IN2
- Unsaturation other than maximum . IN5
- Maximum unsaturation IN9

C_4O
- Complete saturation IP2
- Unsaturation other than maximum . IP5
- Maximum unsaturation IP9

4-membered rings

CO_3
- Complete saturation IS2
- Unsaturation other than maximum . IS5
- Maximum unsaturation IS9

C_2O_2
- Complete saturation IT2
- Unsaturation other than maximum . IT5
- Maximum unsaturation IT9

C_3O
- Complete saturation IV2
- Unsaturation other than maximum . IV5
- Maximum unsaturation IV9

3-membered rings

CO_2
- Saturated IW2
- Unsaturated. IW9

C_2O
- Saturated IX2
- Unsaturated. IX9

(CH)S - NONCYCLIC GROUPS*

Trithiocarbonates	HSC(:S)SH	J15
Carbodithioates	HC(:S)SH	J20
Thiones	RC(:S)R'	J51
Thioaldehydes	HC(:S)H	J55
Nonketonic thiocarbonyl groups	-C(:S)-	J59
Polysulfides	HS_xH (x > 2)	J60
Disulfides	RSSR	J62
	HSSH	J63
Sulfides	R-S	J65
	RSR'	J66
Thiols	RSH	J72
Sulfonium compounds	RH_2S^+, R-SH^+, R-S^+ or R:S^+ (: may be resonating double bond)	J90

CS(Z) RINGS

CSZ

9- or more-membered rings	
Complete saturation	K0K
Unsaturation other than maximum	K0N
Maximum unsaturation	K0R
8-membered rings	
Complete saturation	K12
Unsaturation other than maximum	K15
Maximum unsaturation	K19
7-membered rings	
Complete saturation	K1K
Unsaturation other than maximum	K1N
Maximum unsaturation	K1R
6-membered rings	
Complete saturation	K22
Unsaturation other than maximum	K25
Maximum unsaturation	K29
5-membered rings	
Complete saturation	K2K
Unsaturation other than maximum	K2N
Maximum unsaturation	K2R
4-membered rings	
Complete saturation	K32
Unsaturation other than maximum	K35
Maximum unsaturation	K39
3-membered rings	
Saturated	K3K
Unsaturated	K3R

CS

10- or more-membered rings	
Complete saturation	K42
Unsaturation other than maximum	K45
Maximum unsaturation	K49
9-membered rings	
Complete saturation	K52
Unsaturation other than maximum	K55
Maximum unsaturation	K59
8-membered rings	
Complete saturation	K62
Unsaturation other than maximum	K65
Maximum unsaturation	K69
7-membered rings	
CS_6	
Complete saturation	K72
Unsaturation other than maximum	K75
Maximum unsaturation	K79
C_2S_5	
Complete saturation	K7K
Unsaturation other than maximum	K7N
Maximum unsaturation	K7R
C_3S_4	
Complete saturation	K82
Unsaturation other than maximum	K85
Maximum unsaturation	K89
C_4S_3	
Complete saturation	K8K
Unsaturation other than maximum	K8N
Maximum unsaturation	K8R

* This includes fragments of heterocyclic rings containing a part of the group outside of the ring.

C_5S_2
- Complete saturation K92
- Unsaturation other than maximum . K95
- Maximum unsaturation K99

C_6S
- Complete saturation K9K
- Unsaturation other than maximum . K9N
- Maximum unsaturation K9R

6-membered rings

CS_5
- Complete saturation KA2
- Unsaturation other than maximum . KA5
- Maximum unsaturation KA9

C_2S_4
- Complete saturation KB2
- Unsaturation other than maximum . KB5
- Maximum unsaturation KB9

C_3S_3
- Complete saturation KD2
- Unsaturation other than maximum . KD5
- Maximum unsaturation KD9

C_4S_2
- Complete saturation KF2
- Unsaturation other than maximum . KF5
- Maximum unsaturation KF9

C_5S
- Complete saturation KH2
- Unsaturation other than maximum . KH5
- Maximum unsaturation KH9

5-membered rings

CS_4
- Complete saturation KJ2
- Unsaturation other than maximum . KJ5
- Maximum unsaturation KJ9

C_2S_3
- Complete saturation KL2
- Unsaturation other than maximum . KL5
- Maximum unsaturation KL9

C_3S_2
- Complete saturation KN2
- Unsaturation other than maximum . KN5
- Maximum unsaturation KN9

C_4S
- Complete saturation KP2
- Unsaturation other than maximum . KP5
- Maximum unsaturation KP9

4-membered rings

CS_3
- Complete saturation KS2
- Unsaturation other than maximum . KS5
- Maximum unsaturation KS9

C_2S_2
- Complete saturation KT2
- Unsaturation other than maximum . KT5
- Maximum unsaturation KT9

C_3S
- Complete saturation KV2
- Unsaturation other than maximum . KV5
- Maximum unsaturation KV9

3-membered rings

CS_2
- Saturated KW2
- Unsaturated KW9

C_2S
- Saturated KX2
- Unsaturated KX9

(CH)X

Iodonium or other halonium compounds . . . . RHI^+, $\underline{R\text{-}I}^+$, RHX^+ or $\underline{R\text{-}X}^+$ L14

Iododihalides or other halohalides . . . . . RIX_2, or RX_n ($n > 2$) L19

Fluoro compounds . . . . . RF
- R is heterocyclic L22
- R is aromatic carbocyclic L25
- R is alicyclic or aliphatic L27
- R is unspecified L29

Chloro compounds . . . . . RCl
- R is heterocyclic L32
- R is aromatic carbocyclic L35
- R is alicyclic or aliphatic L37
- R is unspecified L39

Bromo compounds . . . . . RBr
- R is heterocyclic L42
- R is aromatic carbocyclic L45
- R is alicyclic or aliphatic L47
- R is unspecified L49

Iodo compounds . . . . . RI
R is heterocyclic L52
R is aromatic carbocyclic L55
R is alicyclic or aliphatic L57
R is unspecified L59

Halo compounds (unspecified) . . . . . RX L69

CZ RINGS

10- or more-membered rings
Complete saturation M12
Unsaturation other than maximum . M15
Maximum unsaturation M19

9-membered rings
Complete saturation M22
Unsaturation other than maximum . M25
Maximum unsaturation M29

8-membered rings
CZ_7
Complete saturation M32
Unsaturation other than maximum . M35
Maximum unsaturation M39
C_2Z_6
Complete saturation M3K
Unsaturation other than maximum . M3N
Maximum unsaturation M3R
C_3Z_5
Complete saturation M42
Unsaturation other than maximum . M45
Maximum unsaturation M49
C_4Z_4
Complete saturation M4K
Unsaturation other than maximum . M4N
Maximum unsaturation M4R
C_5Z_3
Complete saturation M52
Unsaturation other than maximum . M55
Maximum unsaturation M59
C_6Z_2
Complete saturation M5K
Unsaturation other than maximum . M5N
Maximum unsaturation M5R
C_7Z
Complete saturation M62
Unsaturation other than maximum . M65
Maximum unsaturation M69

7-membered rings
CZ_6
Complete saturation M72
Unsaturation other than maximum . M75
Maximum unsaturation M79
C_2Z_5
Complete saturation M7K
Unsaturation other than maximum . M7N
Maximum unsaturation M7R
C_3Z_4
Complete saturation M82
Unsaturation other than maximum . M85
Maximum unsaturation M89
C_4Z_3
Complete saturation M8K
Unsaturation other than maximum . M8N
Maximum unsaturation M8R
C_5Z_2
Complete saturation M92
Unsaturation other than maximum . M95
Maximum unsaturation M99
C_6Z
Complete saturation M9K
Unsaturation other than maximum . M9N
Maximum unsaturation M9R

6-membered rings
CZ_5
Complete saturation MA2
Unsaturation other than maximum . MA5
Maximum unsaturation MA9
C_2Z_4
Complete saturation MB2
Unsaturation other than maximum . MB5
Maximum unsaturation MB9
C_3Z_3
Complete saturation MD2
Unsaturation other than maximum . MD5
Maximum unsaturation MD9
C_4Z_2
Complete saturation MF2
Unsaturation other than maximum . MF5
Maximum unsaturation MF9
C_5Z
Complete saturation MH2
Unsaturation other than maximum . MH5
Maximum unsaturation MH9

5-membered rings
CZ_4
Complete saturation MJ2
Unsaturation other than maximum . MJ5
Maximum unsaturation MJ9

C_2Z_3
- Complete saturation ML2
- Unsaturation other than maximum . ML5
- Maximum unsaturation ML9

C_3Z_2
- Complete saturation MN2
- Unsaturation other than maximum . MN5
- Maximum unsaturation MN9

C_4Z
- Complete saturation MP2
- Unsaturation other than maximum . MP5
- Maximum unsaturation MP9

4-membered rings

CZ_3
- Complete saturation MS2
- Unsaturation other than maximum . MS5
- Maximum unsaturation MS9

C_2Z_2
- Complete saturation MT2
- Unsaturation other than maximum . MT5
- Maximum unsaturation MT9

C_3Z
- Complete saturation MV2
- Unsaturation other than maximum . MV5
- Maximum unsaturation MV9

3-membered rings

CZ_2
- Saturated MW2
- Unsaturated MW9

C_2Z
- Saturated MX2
- Unsaturated MX9

C RINGS

10- or more-fused-ring systems. N00

9-fused-ring systems. N01

8-fused-ring systems. N02

7-fused-ring systems. N03

6-fused-ring systems. N04

5-fused-ring systems. N05

4-fused-ring systems

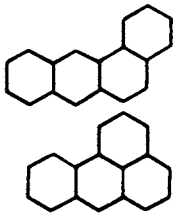
7+,7+,7+,7+
- Complete saturation. N12
- Unsaturation other than maximum . . . N15
- Maximum conjugated unsaturation . . . N19

6,7+,7+,7+
- Complete saturation. N1B
- Unsaturation other than maximum . . . N1E
- Maximum conjugated unsaturation . . . N1I

6,6,7+,7+
- Complete saturation N1K
- Unsaturation other than maximum . . . N1N
- Maximum conjugated unsaturation . . . N1R

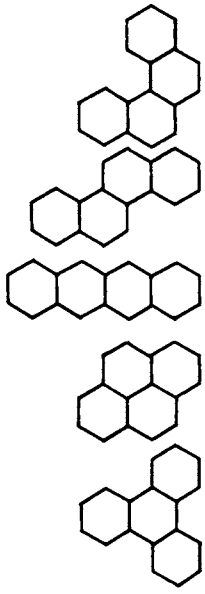
6,6,6,7+
- Complete saturation. N1S
- Unsaturation other than maximum . . . N1V
- Maximum conjugated unsaturation . . . N1Z

6,6,6,6



Benz[a]anthracene
- Complete saturation N22
- Unsaturation other than maximum . . . N25
- Maximum conjugated unsaturation (9) . N29

Benz[de]anthracene
- Complete saturation N2B
- Unsaturation other than maximum . . . N2E
- Maximum conjugated unsaturation (8) . N2I



Benzo[c]phenanthrene
- Complete saturation. N2K
- Unsaturation other than maximum . . . N2N
- Maximum conjugated unsaturation (9) . N2R

Chrysene
- Complete saturation. N32
- Unsaturation other than maximum . . . N35
- Maximum conjugated unsaturation (9) . N39

Naphthacene
- Complete saturation N3B
- Unsaturation other than maximum . . . N3E
- Maximum conjugated unsaturation (9) . N3I

Pyrene
- Complete saturation. N3K
- Unsaturation other than maximum . . . N3N
- Maximum conjugated unsaturation (8) . N3R

Triphenylene
- Complete saturation. N42
- Unsaturation other than maximum . . . N45
- Maximum conjugated unsaturation (9) . N49

Others
- Complete saturation. N4B
- Unsaturation other than maximum . . . N4E
- Maximum conjugated unsaturation . . . N4I

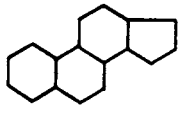
5,7+,7+,7+
- Complete saturation. N52
- Unsaturation other than maximum . . . N55
- Maximum conjugated unsaturation . . . N59

5,6,7+,7+
- Complete saturation. N5B
- Unsaturation other than maximum . . . N5E
- Maximum conjugated unsaturation . . . N5I

5,6,6,7+
- Complete saturation. N5K
- Unsaturation other than maximum . . . N5N
- Maximum conjugated unsaturation . . . N5R

5,6,6,6

Cyclopenta[a]phenanthrene
- Complete saturation. N62
- One unsaturation N63
- Two unsaturations N64
- Three or four unsaturations N65
- Five unsaturations N66
- Six unsaturations N67
- Seven unsaturations N68
- Maximum conjugated unsaturation (8) . N69



Others
- Complete saturation. N6S
- Unsaturation other than maximum . . . N6V
- Maximum conjugated unsaturation . . . N6Z

5,5,7+,7+
- Complete saturation. N72
- Unsaturation other than maximum . . . N75
- Maximum conjugated unsaturation . . . N79

5,5,6,7+
- Complete saturation. N7B
- Unsaturation other than maximum . . . N7E
- Maximum conjugated unsaturation . . . N7I

5,5,6,6
- Complete saturation. N7K
- Unsaturation other than maximum . . . N7N
- Maximum conjugated unsaturation . . . N7R

5,5,5,7+
- Complete saturation. N7S
- Unsaturation other than maximum . . . N7V
- Maximum conjugated unsaturation . . . N7Z

5,5,5,6
- Complete saturation. N82
- Unsaturation other than maximum . . . N85
- Maximum conjugated unsaturation . . . N89

5,5,5,5
- Complete saturation. N8B
- Unsaturation other than maximum . . . N8E
- Maximum conjugated unsaturation . . . N8I

4,7+,7+,7+
- Complete saturation. N8K
- Unsaturation other than maximum . . . N8N
- Maximum conjugated unsaturation . . . N8R

4,6,7+,7+
- Complete saturation. N8S
- Unsaturation other than maximum . . . N8V
- Maximum conjugated unsaturation . . . N8Z

4,6,6,7+
- Complete saturation. N92
- Unsaturation other than maximum . . . N95
- Maximum conjugated unsaturation . . . N99

4,6,6,6
- Complete saturation. N9B
- Unsaturation other than maximum . . . N9E
- Maximum conjugated unsaturation . . . N9I

4,5,7+,7+
- Complete saturation. N9K
- Unsaturation other than maximum . . . N9N
- Maximum conjugated unsaturation . . . N9R

4,5,6,7+
- Complete saturation. N9S
- Unsaturation other than maximum . . . N9V
- Maximum conjugated unsaturation . . . N9Z

4,5,6,6
- Complete saturation. NA2
- Unsaturation other than maximum . . . NA5
- Maximum conjugated unsaturation . . . NA9

4,5,5,7+
- Complete saturation. . . . . NAB
- Unsaturation other than maximum . . . NAE
- Maximum conjugated unsaturation . . . NAI

4,5,5,6
- Complete saturation. . . . . NAK
- Unsaturation other than maximum . . . NAN
- Maximum conjugated unsaturation . . . NAR

4,5,5,5
- Complete saturation. . . . . NAS
- Unsaturation other than maximum . . . NAV
- Maximum conjugated unsaturation . . . NAZ

4,4,7+,7+
- Complete saturation. NB2
- Unsaturation other than maximum . . . NB5
- Maximum conjugated unsaturation . . . NB9

4,4,6,7+
- Complete saturation. . . . . NBB
- Unsaturation other than maximum . . . NBE
- Maximum conjugated unsaturation . . . NBI

4,4,6,6
- Complete saturation. . . . . NBK
- Unsaturation other than maximum . . . NBN
- Maximum conjugated unsaturation . . . NBR

4,4,5,7+
- Complete saturation. . . . . NBS
- Unsaturation other than maximum . . . NBV
- Maximum conjugated unsaturation . . . NBZ

4,4,5,6
- Complete saturation. NC2
- Unsaturation other than maximum . . . NC5
- Maximum conjugated unsaturation . . . NC9

4,4,5,5
- Complete saturation. . . . . NCB
- Unsaturation other than maximum . . . NCE
- Maximum conjugated unsaturation . . . NCI

4,4,4,7+
- Complete saturation. . . . . NCK
- Unsaturation other than maximum . . . NCN
- Maximum conjugated unsaturation . . . NCR

4,4,4,6
- Complete saturation. . . . . NCS
- Unsaturation other than maximum . . . NCV
- Maximum conjugated unsaturation . . . NCZ

4,4,4,5
- Complete saturation. ND2
- Unsaturation other than maximum . . . ND5
- Maximum conjugated unsaturation . . . ND9

4,4,4,4
- Complete saturation. . . . . NDB
- Unsaturation other than maximum . . . NDE
- Maximum conjugated unsaturation . . . NDI

3,7+,7+,7+
- Complete saturation. . . . . NDK
- Unsaturation other than maximum . . . NDN
- Maximum conjugated unsaturation . . . NDR

3,6,7+,7+
- Complete saturation. . . . . NDS
- Unsaturation other than maximum . . . NDV
- Maximum conjugated unsaturation . . . NDZ

3,6,6,7+
- Complete saturation. NE2
- Unsaturation other than maximum . . . NE5
- Maximum conjugated unsaturation . . . NE9

3,6,6,6
- Complete saturation. . . . . NEB
- Unsaturation other than maximum . . . NEE
- Maximum conjugated unsaturation . . . NEI

3,5,7+,7+
- Complete saturation. . . . . NEK
- Unsaturation other than maximum . . . NEN
- Maximum conjugated unsaturation . . . NER

3,5,6,7+
- Complete saturation. . . . . NES
- Unsaturation other than maximum . . . NEV
- Maximum conjugated unsaturation . . . NEZ

3,5,6,6
- Complete saturation. NF2
- Unsaturation other than maximum . . . NF5
- Maximum conjugated unsaturation . . . NF9

3,5,5,7+
- Complete saturation. . . . . NFB
- Unsaturation other than maximum . . . NFE
- Maximum conjugated unsaturation . . . NFI

3,5,5,6
- Complete saturation. . . . . NFK
- Unsaturation other than maximum . . . NFN
- Maximum conjugated unsaturation . . . NFR

3,5,5,5
- Complete saturation. . . . . NFS
- Unsaturation other than maximum . . . NFV
- Maximum conjugated unsaturation . . . NFZ

3,4,7+,7+
- Complete saturation. NG2
- Unsaturation other than maximum . . . NG5
- Maximum conjugated unsaturation . . . NG9

3,4,6,7+
- Complete saturation. . . . . NGB
- Unsaturation other than maximum . . . NGE
- Maximum conjugated unsaturation . . . NGI

3,4,6,6
- Complete saturation. . . . . NGK
- Unsaturation other than maximum . . . NGN
- Maximum conjugated unsaturation . . . NGR

3,4,5,7+
- Complete saturation. . . . . NGS
- Unsaturation other than maximum . . . NGV
- Maximum conjugated unsaturation . . . NGZ

3,4,5,6
- Complete saturation. NH2
- Unsaturation other than maximum . . . NH5
- Maximum conjugated unsaturation . . . NH9

3,4,5,5
- Complete saturation. . . . . NHB
- Unsaturation other than maximum . . . NHE
- Maximum conjugated unsaturation . . . NHI

3,4,4,7+
- Complete saturation. . . . . NHK
- Unsaturation other than maximum . . . NHN
- Maximum conjugated unsaturation . . . NHR

3,4,4,6
- Complete saturation. . . . . NHS
- Unsaturation other than maximum . . . NHV
- Maximum conjugated unsaturation . . . NHZ

3,4,4,5
- Complete saturation. NI2
- Unsaturation other than maximum . . . NI5
- Maximum conjugated unsaturation . . . NI9

3,4,4,4
- Complete saturation. . . . . NIB
- Unsaturation other than maximum . . . NIE
- Maximum conjugated unsaturation . . . NII

4-fused-ring systems with two or more rings of three numbers
- Complete saturation. . . . . NIS
- Unsaturation other than maximum . . . NIV
- Maximum conjugated unsaturation . . . NIZ

3-fused-ring systems

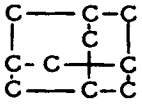
7+,7+,7+
- Complete saturation. NJ2
- Unsaturation other than maximum . . . NJ5
- Maximum conjugated unsaturation . . . NJ9

6,7+,7+
- Complete saturation. . . . . NJB
- Unsaturation other than maximum . . . NJE
- Maximum conjugated unsaturation . . . NJI

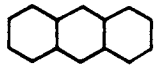
6,6,7+
- Complete saturation. . . . . NJK
- Unsaturation other than maximum . . . NJN
- Maximum conjugated unsaturation . . . NJR

6,6,6

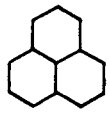
Adamantane



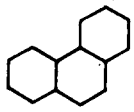
- Complete saturation. NK2
- Unsaturation other than maximum . . . NK5
- Maximum conjugated unsaturation (4) . NK9



Anthracene
- Complete saturation. . . . . NKB
- One unsaturation . . . . . NKC
- Two unsaturations. . . . . NKD
- Three unsaturations . . . . . NKE
- Four unsaturations . . . . . NKF
- Five unsaturations . . . . . NKG
- Six unsaturations . . . . . NKH
- Maximum conjugated unsaturation (7) . NKI



Benzonaphthene
- Complete saturation. . . . . NKK
- One unsaturation . . . . . NKL
- Two unsaturations. . . . . NKM
- Three unsaturations. . . . . NKN
- Four unsaturations . . . . . NKØ
- Five unsaturations . . . . . NKP
- Maximum conjugated unsaturation (6) . NKR



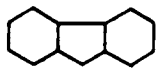
Phenanthrene
- Complete saturation. NL2
- One unsaturation NL3
- Two unsaturations NL4
- Three unsaturations. NL5
- Four unsaturations NL6
- Five unsaturations NL7
- Six unsaturations NL8
- Maximum conjugated unsaturation (7) . NL9

Others
- Complete saturation. . . . . NLB
- Unsaturation other than maximum . . . NLE
- Maximum conjugated unsaturation . . . NLI

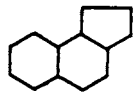
5,7+,7+
- Complete saturation. NM2
- Unsaturation other than maximum . . . NM5
- Maximum conjugated unsaturation . . . NM9

5,6,7+
- Complete saturation. . . . . NMB
- Unsaturation other than maximum . . . NME
- Maximum conjugated unsaturation . . . NMI

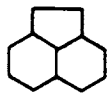
5,6,6



Fluorene
- Complete saturation. NN2
- Unsaturation other than maximum . . . NN5
- Maximum conjugated unsaturation (6) . NN9



Benz[e]indene
- Complete saturation. . . . . NNB
- Unsaturation other than maximum . . . NNE
- Maximum conjugated unsaturation (6) . NNI



Acenaphthylene
- Complete saturation. . . . . NNK
- Unsaturation other than maximum . . . NNN
- Maximum conjugated unsaturation (6) . NNR

Others
- Complete saturation. . . . . NNS
- Unsaturation other than maximum . . . NNV
- Maximum conjugated unsaturation . . . NNZ

5,5,7+
- Complete saturation. NØ2
- Unsaturation other than maximum . . . NØ5
- Maximum conjugated unsaturation . . . NØ9

5,5,6
- Complete saturation. . . . . NØB
- Unsaturation other than maximum . . . NØE
- Maximum conjugated unsaturation . . . NØI

5,5,5
- Complete saturation. . . . . NØK
- Unsaturation other than maximum . . . NØN
- Maximum conjugated unsaturation . . . NØR

4,7+,7+
- Complete saturation. . . . . NØS
- Unsaturation other than maximum . . . NØV
- Maximum conjugated unsaturation . . . NØZ

4,6,7+
- Complete saturation. NP2
- Unsaturation other than maximum . . . NP5
- Maximum conjugated unsaturation . . . NP9

4,6,6
- Complete saturation. . . . . NPB
- Unsaturation other than maximum . . . NPE
- Maximum conjugated unsaturation . . . NPI

4,5,7+
- Complete saturation. . . . . NPK
- Unsaturation other than maximum . . . NPN
- Maximum conjugated unsaturation . . . NPR

4,5,6
- Complete saturation . . . . . NPS
- Unsaturation other than maximum . . . NPV
- Maximum conjugated unsaturation . . . NPZ

4,5,5
- Complete saturation. NQ2
- Unsaturation other than maximum . . . NQ5
- Maximum conjugated unsaturation . . . NQ9

4,4,7+
- Complete saturation. . . . . NQB
- Unsaturation other than maximum . . . NQE
- Maximum conjugated unsaturation . . . NQI

4,4,6
- Complete saturation. . . . . NQK
- Unsaturation other than maximum . . . NQN
- Maximum conjugated unsaturation . . . NQR

4,4,5
- Complete saturation. . . . . NQS
- Unsaturation other than maximum . . . NQV
- Maximum conjugated unsaturation . . . NQZ

4,4,4
- Complete saturation. NR2
- Unsaturation other than maximum . . . NR5
- Maximum conjugated unsaturation . . . NR9

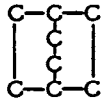
3-fused-ring systems with one or more rings of three members
- Complete saturation. . . . . NRS
- Unsaturation other than maximum . . . NRV
- Maximum conjugated unsaturation . . . NRZ

2-fused-ring systems

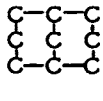
7+,7+
- Complete saturation. NS2
- Unsaturation other than maximum . . . NS5
- Maximum conjugated unsaturation . . . NS9

6,7+
- Complete saturation. . . . . NSB
- Unsaturation other than maximum . . . NSE
- Maximum conjugated unsaturation . . . NSI

6,6

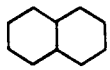


Bicyclo[2.2.2]octane
- Complete saturation. NT2
- Unsaturation other than maximum . . . NT5
- Maximum conjugated unsaturation (4) . NT9



Bicyclo[3.3.1]nonane
- Complete saturation. . . . . NTB
- Unsaturation other than maximum . . . NTE
- Maximum conjugated unsaturation (4) . NTI

Naphthalene

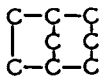


Complete saturation. . . . . NTK
One unsaturation . . . . . NTL
Two unsaturations . . . . . NTM
Three unsaturations. . . . . NTN
Four unsaturations . . . . . NTØ
Maximum conjugated unsaturation (5) . NTR

5,7+

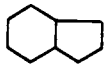
Complete saturation. NU2
Unsaturation other than maximum . . . NU5
Maximum conjugated unsaturation . . . NU9

5,6



Bicyclo[3.2.1]octane
Complete saturation. NV2
Unsaturation other than maximum . . . NV5
Maximum conjugated unsaturation (4) . NV9

Indene



Complete saturation. . . . . NVB
Unsaturation other than maximum . . . NVE
Maximum conjugated unsaturation (4) . NVI

5,5

Complete saturation. NW2
Unsaturation other than maximum . . . NW5
Maximum conjugated unsaturation . . . NW9

4,7+

Complete saturation. . . . . NWB
Unsaturation other than maximum . . . NWE
Maximum conjugated unsaturation . . . NWI

4,6

Complete saturation. . . . . NWK
Unsaturation other than maximum . . . NWN
Maximum conjugated unsaturation . . . NWR

4,5

Complete saturation. . . . . NWS
Unsaturation other than maximum . . . NWV
Maximum conjugated unsaturation . . . NWZ

4,4

Complete saturation. NX2
Unsaturation other than maximum . . . NX5
Maximum conjugated unsaturation . . . NX9

2-fused-ring systems with one or two rings of three members

Complete saturation. . . . . NXS
Unsaturation other than maximum . . . NXV
Maximum conjugated unsaturation . . . NXZ

1-ring systems

7+

Complete saturation. NY2
Unsaturation other than maximum . . . NY5
Maximum conjugated unsaturation . . . NY9

6

Cyclohexane* . . . . . NYB
Cyclohexene* . . . . . NYC
Cyclohexadiene* . . . . . NYD
Benzene* . . . . . NYI
Cyclohexane . . . . . NYK
Cyclohexene . . . . . NYL
Cyclohexadiene . . . . . NYM
Benzene . . . . . NYR

* Fused to heterocyclic structures

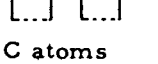
5
- Complete saturation. NZ2
- Unsaturation other than maximum . . . NZ5
- Maximum conjugated unsaturation (2) . NZ9

4
- Complete saturation. . . . . NZB
- Unsaturation other than maximum . . . NZE
- Maximum conjugated unsaturation (2) . NZI

3
- Saturated . . . . . NZK
- Unsaturated . . . . . NZR

Unspecified cyclic hydrocarbon structures . . . NZZ

C(H) - NONCYCLIC GROUPS

Carbon to carbon double bonds which are intercyclic or between cyclic and noncyclic structures  or  Ø08

21 or more C atoms
- Unsaturated Ø28
- Saturated. Ø29

20 C atoms
- Double and triple bonds Ø34
- Triple bonds only Ø35
- Three or more double bonds Ø36
- Two double bonds Ø37
- One double bond Ø38
- Saturated. Ø39

19 C atoms
- Double and triple bonds Ø3D
- Triple bonds only Ø3E
- Three or more double bonds Ø3F
- Two double bonds Ø3G
- One double bond Ø3H
- Saturated Ø3I

18 C atoms
- Double and triple bonds Ø3M
- Triple bonds only Ø3N
- Three or more double bonds Ø3Ø
- Two double bonds Ø3P
- One double bond Ø3Q
- Saturated Ø3R

17 C atoms
- Double and triple bonds Ø3U
- Triple bonds only Ø3V
- Three or more double bonds Ø3W
- Two double bonds Ø3X
- One double bond Ø3Y
- Saturated Ø3Z

16 C atoms
- Double and triple bonds Ø44
- Triple bonds only Ø45
- Three or more double bonds Ø46
- Two double bonds Ø47
- One double bond Ø48
- Saturated. Ø49

15 C atoms
- Double and triple bonds Ø4D
- Triple bonds only Ø4E
- Three or more double bonds Ø4F
- Two double bonds Ø4G
- One double bond Ø4H
- Saturated. Ø4I

14 C atoms
- Double and triple bonds Ø4M
- Triple bonds only Ø4N
- Three or more double bonds Ø4Ø
- Two double bonds Ø4P
- One double bond Ø4Q
- Saturated. Ø4R

13 C atoms
- Double and triple bonds Ø4U
- Triple bonds only Ø4V
- Three or more double bonds Ø4W
- Two double bonds Ø4X
- One double bond Ø4Y
- Saturated. Ø4Z

12 C atoms
- Double and triple bonds Ø54
- Triple bonds only Ø55
- Three or more double bonds Ø56
- Two double bonds Ø57
- One double bond Ø58
- Saturated. Ø59

11 C atoms
- Double and triple bonds Ø5D
- Triple bonds only Ø5E
- Three or more double bonds Ø5F
- Two double bonds Ø5G
- One double bond Ø5H
- Saturated. Ø5I

10 C atoms
- Double and triple bonds Ø5M
- Triple bonds only Ø5N
- Three or more double bonds Ø5Ø
- Two double bonds Ø5P
- One double bond Ø5Q
- Saturated. Ø5R

9 C atoms
- Double and triple bonds Ø5U
- Triple bonds only Ø5V
- Three or more double bonds Ø5W
- Two double bonds Ø5X
- One double bond Ø5Y
- Saturated Ø5Z

8 C atoms
- Double and triple bonds Ø64
- Triple bonds only Ø65
- Three or more double bonds Ø66
- Two double bonds Ø67
- One double bond Ø68
- Saturated. Ø69

7 C atoms
- Double and triple bonds Ø6D
- Triple bonds only Ø6E
- Three or more double bonds Ø6F
- Two double bonds Ø6G
- One double bond Ø6H
- Saturated Ø6I

6 C atoms
- Two triple and one double bond Ø6K
- One triple and three double bonds. . . Ø6L
- One triple and two double bonds . . . Ø6M
- One triple and one double bond Ø6N
- Three triple bonds Ø6Ø
- Two triple bonds. Ø6S
- One triple bond Ø6T
- Five double bonds Ø6U
- Four double bonds Ø6V
- Three double bonds Ø6W
- Two double bonds Ø6X
- One double bond Ø6Y
- Saturated. Ø6Z

5 C atoms
- One triple and two double bonds . . Ø7A
- One triple and one double bond . . . Ø7B
- Two triple bonds. Ø7C
- One triple bond Ø7D
- Four double bonds Ø7E
- Three double bonds Ø7F
- Two double bonds Ø7G
- One double bond Ø7H
- Saturated. Ø7I

4 C atoms
- One triple and one double bond . . . Ø7L
- Two triple bonds Ø7M
- One triple bond Ø7N
- Three double bonds Ø7Ø
- Two double bonds Ø7P
- One double bond Ø7Q
- Saturated. Ø7R

3 C atoms
- One triple bond Ø7W
- Two double bonds Ø7X
- One double bond Ø7Y
- Saturated. Ø7Z

2 C atoms
- One triple bond Ø86
- One double bond Ø88
- Saturated Ø89

1 C atom Ø99

Unspecified noncyclic hydrocarbon structures. . . . . ØZZ

DIVISION II - ORGANOHETEROID GROUPS*

FAMILY P--

Ac (Actinium)
- Ac chain . . . P0(12)
- Ac^3 . . . . . P0E
- Ac° P0H

Ag (Silver)
- Ag chain . . . P0(11)
- Ag^3 . . . . . P0M
- Ag^2 . . . . . P0N
- Ag^1 . . . . . P0Ø
- Ag° P0P

Al (Aluminum)
- Al chain . . . P10
- Al^3 . . . . . P12
- Al° P15

Am (Americium)
- Am chain. . . P1(12)
- Am^3 . . . . . P1E
- Am° P1H

As (Arsenic)
- As chain . . . P1(11)
- As^5 . . . . . P1J
- As^4 . . . . . P1K
- As^3 . . . . . P1L
- As^2 . . . . . P1M
- As° P1Ø

At (Astatine)
- At chain . . . P20
- At° P28

Au (Gold)
- Au chain . . . P2(12)
- Au^3 . . . . . P2D
- Au^2 . . . . . P2E
- Au^1 . . . . . P2F
- Au° P2G

B (Boron)
- B chain. . . . P2(11)
- B^3 . . . . . P2K
- B° P2N

Ba (Barium)
- Ba chain . . . P30
- Ba^2 . . . . . P35
- Ba° P37

Be (Beryllium)
- Be chain . . . P3(12)
- Be^2 . . . . . P3E
- Be° P3G

Bi (Bismuth)
- Bi chain . . . P3(11)
- Bi^5 . . . . . P3J
- Bi^4 . . . . . P3K
- Bi^3 . . . . . P3L
- Bi^2 . . . . . P3M
- Bi° P3Ø

Ca (Calcium)
- Ca chain . . . P4(11)
- Ca^2 . . . . . P4N
- Ca° P4P

Cb (Columbium)
- Cb chain . . . P50
- Cb^5 . . . . . P51
- Cb^4 . . . . . P52
- Cb^3 . . . . . P53
- Cb^2 . . . . . P54
- Cb° P56

Cd (Cadmium)
- Cd chain . . . P5(12)
- Cd^2 . . . . . P5E
- Cd° P5G

Ce (Cerium)
- Ce chain . . . P5(11)
- Ce^4 . . . . . P5K
- Ce^3 . . . . . P5L
- Ce° P5Ø

Cm (Curium)
- Cm chain . . P6(12)
- Cm^3 . . . . . P6E
- Cm° P6H

Co (Cobalt)
- Co chain . . . P6(11)
- Co^4 . . . . . P6N
- Co^3 . . . . . P6Ø
- Co^2 . . . . . P6P
- Co° P6R

Cr (Chromium)
- Cr chain . . . P70
- Cr^6 . . . . . P72
- Cr^4 . . . . . P74
- Cr^3 . . . . . P75
- Cr^2 . . . . . P76
- Cr^1 . . . . . P77
- Cr° P78

Cs (Cesium)
- Cs chain . . . P7(12)
- Cs^1 . . . . . P7F
- Cs° P7G

Cu (Copper)
- Cu chain . . . P7(11)
- Cu^3 . . . . . P7M
- Cu^2 . . . . . P7N
- Cu^1 . . . . . P7Ø
- Cu° P7P

Dy (Dysprosium)
- Dy chain . . . P80
- Dy^3 . . . . . P83
- Dy° P86

Er (Erbium)
- Er chain . . . P8(12)
- Er^3 . . . . . P8C
- Er° P8F

Eu (Europium)
- Eu chain . . . P8(11)
- Eu^3 . . . . . P8L
- Eu^2 . . . . . P8M
- Eu° P8Ø

Fa (Francium)
- Fa chain . . . P9(12)
- Fa^1 . . . . . P9F
- Fa° P9G

Fe (Iron)
- Fe chain . . . P9(11)
- Fe^6 . . . . . P9L
- Fe^4 . . . . . P9N
- Fe^3 . . . . . P9Ø
- Fe^2 . . . . . P9P
- Fe° P9R

* Superscripts are combining powers of the elements (See p. 24, Sec. 6.1); superscript (°) is included for reference.

Ga (Gallium)
- Ga chain . . . PA0
- Ga^3 . . . . . PA2
- Ga^2 . . . . . PA3
- Ga° PA5

Gd (Gadolinium)
- Gd chain . . . PA(12)
- Gd^3 . . . . . PAC
- Gd° . . . . . PAF

Ge (Germanium)
- Ge chain . . . PA(11)
- Ge^4 . . . . . PAJ
- Ge^2 . . . . . PAL
- Ge° . . . . . PAN

Hf (Hafnium)
- Hf chain . . . PB(11)
- Hf^4 . . . . . PBJ
- Hf° . . . . . PBN

Hg (Mercury)
- Hg chain . . . PC0
- Hg^2 . . . . . PC5
- Hg^1 . . . . . PC6
- Hg° PC7

Ho (Holmium)
- Ho chain . . . PC(12)
- Ho^3 . . . . . PCC
- Ho° . . . . . PCF

In (Indium)
- In chain . . . PD0
- In^3 . . . . . PD2
- In° PD5

Ir (Iridium)
- Ir chain . . . PD(12)
- Ir^6 . . . . . PDC
- Ir^4 . . . . . PDE
- Ir^3 . . . . . PDF
- Ir^2 . . . . . PDG
- Ir° . . . . . PDI

K (Potassium)
- K chain. . . . PD(11)
- K^1 . . . . . PDØ
- K° . . . . . PDP

La (Lanthanum)
- La chain . . . PE(12)
- La^3 . . . . . PEC
- La° . . . . . PEF

Li (Lithium)
- Li chain . . . PE(11)
- Li^1 . . . . . PEØ
- Li° . . . . . PEP

Lu (Lutetium)
- Lu chain . . . PF0
- Lu^3 . . . . . PF3
- Lu° PF6

Mg (Magnesium)
- Mg chain . . . PF(12)
- Mg^2 . . . . . PFE
- Mg° . . . . . PFG

Mn (Manganese)
- Mn chain . . . PF(11)
- Mn^7 . . . . . PFJ
- Mn^6 . . . . . PFK
- Mn^4 . . . . . PFM
- Mn^3 . . . . . PFN
- Mn^2 . . . . . PFØ
- Mn^1 . . . . . PFP
- Mn° . . . . . PFQ

Mo (Molybdenum)
- Mo chain . . . PG0
- Mo^6 . . . . . PG2
- Mo^5 . . . . . PG3
- Mo^4 . . . . . PG4
- Mo^3 . . . . . PG5
- Mo^2 . . . . . PG6
- Mo° PG8

Na (Sodium)
- Na chain . . . PG(11)
- Na^1 . . . . . PGØ
- Na° . . . . . PGP

Nd (Neodymium)
- Nd chain . . . PH0
- Nd^3 . . . . . PH3
- Nd° PH6

Ni (Nickel)
- Ni chain . . . PH(11)
- Ni^6 . . . . . PHL
- Ni^3 . . . . . PHØ
- Ni^2 . . . . . PHP
- Ni^1 . . . . . PHQ
- Ni° . . . . . PHR

Np (Neptunium)
- Np chain . . . PI0
- Np^3 . . . . . PI5
- Np° PI8

Os (Osmium)
- Os chain . . . PI(11)
- Os^8 . . . . . PIJ
- Os^7 . . . . . PIK
- Os^6 . . . . . PIL
- Os^4 . . . . . PIN
- Os^3 . . . . . PIØ
- Os° . . . . . PIR

P (Phosphorus)
- P chain . . . PJ0
- P^5 . . . . . PJ1
- P^4 . . . . . PJ2
- P^3 . . . . . PJ3
- P^2 . . . . . PJ4
- P^1 . . . . . PJ5
- P° PJ6

Pa (Protactinium)
- Pa chain . . . PJ(12)
- Pa^3 . . . . . PJE
- Pa° . . . . . PJH

Pb (Lead)
- Pb chain . . . PJ(11)
- Pb^4 . . . . . PJJ
- Pb^2 . . . . . PJL
- Pb° . . . . . PJN

Pd (Palladium)
- Pd chain . . . PK0
- Pd^4 . . . . . PK5
- Pd^2 . . . . . PK7
- Pd^1 . . . . . PK8
- Pd° PK9

Pm (Promethium)
- Pm chain. . . PV(11)
- Pm^3 . . . . . PVL
- Pm° . . . . . PVØ

Po (Polonium)
- Po chain . . . PK(12)
- Po° . . . . . PKG

Pr (Praseodymium)
- Pr chain . . . PK(11)
- Pr^3 . . . . . PKL
- Pr° . . . . . PKØ

Pt (Platinum)
- Pt chain . . . PL0
- Pt^6 . . . . . PL3
- Pt^5 . . . . . PL4
- Pt^4 . . . . . PL5
- Pt^3 . . . . . PL6
- Pt^2 . . . . . PL7
- Pt° PL9

Pu (Plutonium)
- Pu chain . . . PL(12)
- Pu^6 . . . . . PLB
- Pu^4 . . . . . PLD
- Pu^3 . . . . . PLE
- Pu° . . . . . PLH

Ra (Radium)
- Ra chain . . . PL(11)
- Ra^2 . . . . . PLN
- Ra° . . . . . PLP

Rb (Rubidium)
- Rb chain . . . PM0
- Rb^1 . . . . . PM6
- Rb° PM7

Re (Rhenium)
- Re chain . . . PM(12)
- Re^7 . . . . . PMA
- Re^6 . . . . . PMB
- Re^5 . . . . . PMC
- Re^4 . . . . . PMD
- Re^3 . . . . . PME
- Re° . . . . . PMH

Rh (Rhodium)
- Rh chain . . . PM(11)
- Rh^6 . . . . . PML
- Rh^4 . . . . . PMN
- Rh^3 . . . . . PMØ
- Rh^2 . . . . . PMP
- Rh° . . . . . PMR

Ru (Ruthenium)
- Ru chain . . . PN(12)
- Ru^8 . . . . . PNA
- Ru^7 . . . . . PNB
- Ru^5 . . . . . PND
- Ru^4 . . . . . PNE
- Ru^3 . . . . . PNF
- Ru° . . . . . PNI

Sb (Antimony)
- Sb chain . . . PØ0
- Sb^5 . . . . . PØ1
- Sb^3 . . . . . PØ3
- Sb° PØ6

Sc (Scandium)
- Sc chain . . . PØ(12)
- Sc^3 . . . . . PØC
- Sc° . . . . . PØF

Se (Selenium)
- Se chain . . . PØ(11)
- Se^6 . . . . . PØJ
- Se^4 . . . . . PØL
- Se^2 . . . . . PØN
- Se° . . . . . PØP

Si (Silicon)
- Si chain . . . PP0
- Si^4 . . . . . PP1
- Si° PP5

Sm (Samarium)
- Sm chain . . PP(12)
- Sm^3 . . . . . PPC
- Sm° . . . . . PPF

Sn (Tin)
- Sn chain . . . PP(11)
- Sn^4 . . . . . PPJ
- Sn^2 . . . . . PPL
- Sn° . . . . . PPN

Sr (Strontium)
- Sr chain . . . PQ0
- Sr^2 . . . . . PQ5
- Sr° PQ7

Ta (Tantalum)
- Ta chain . . . PQ(12)
- Ta^5 . . . . . PQA
- Ta^4 . . . . . PQB
- Ta^3 . . . . . PQC
- Ta° . . . . . PQF

Tb (Terbium)
- Tb chain . . . PQ(11)
- Tb^3 . . . . . PQL
- Tb° . . . . . PQØ

Tc (Technetium)
- Tc chain . . . PR0
- Tc° PR8

Te (Tellurium)
- Te chain . . . PR(12)
- Te^6 . . . . . PRA
- Te^4 . . . . . PRC
- Te^2 . . . . . PRE
- Te° . . . . . PRG

Th (Thorium)
- Th chain . . . PR(11)
- Th^4 . . . . . PRM
- Th^3 . . . . . PRN
- Th° . . . . . PRQ

Ti (Titanium)
- Ti chain . . . PS0
- Ti^4 . . . . . PS1
- Ti^3 . . . . . PS2
- Ti^1 . . . . . PS4
- Ti° PS5

Tl (Thallium)
- Tl chain . . . PS(12)
- Tl^3 . . . . . PSB
- Tl^1 . . . . . PSD
- Tl° . . . . . PSE

Tm (Thulium)
- Tm chain . . PS(11)
- Tm^3 . . . . . PSL
- Tm° . . . . . PSØ

U (Uranium)
- U chain. . . . PT0
- U^6 . . . . . PT2
- U^4 . . . . . PT4
- U^3 . . . . . PT5
- U^2 . . . . . PT6
- U^1 . . . . . PT7
- U° PT8

V (Vanadium)
- V chain. . . . PT(12)
- V^5 . . . . . PTA
- V^4 . . . . . PTB
- V^3 . . . . . PTC
- V^2 . . . . . PTD
- V^1 . . . . . PTE
- V° . . . . . PTF

W (Tungsten)
- W chain . . . PT(11)
- W^6 . . . . . PTK
- W^5 . . . . . PTL
- W^4 . . . . . PTM
- W^3 . . . . . PTN
- W^2 . . . . . PTØ
- W° . . . . . PTQ

Y (Yttrium)
- Y chain. . . . PU(12)
- Y^3 . . . . . PUC
- Y° . . . . . PUF

Yb (Ytterbium)
- Yb chain . . . PU(11)
- Yb^3 . . . . . PUL
- Yb^2 . . . . . PUM
- Yb° . . . . . PUØ

Zn (Zinc)
- Zn chain . . . PV0
- Zn^2 . . . . . PV5
- Zn° PV7

Zr (Zirconium)
- Zr chain . . . PV(12)
- Zr^4 . . . . . PVA
- Zr° . . . . . PVE

Unspecified
- Unspecified element. . . PZZ (other than C,H,N,O, S or X linked to carbon)

DIVISION III - INORGANIC GROUPS

FAMILIES Q-- to V--

RINGS CONTAINING NO CARBON

3-membered rings containing:
- One element Q31
- Two elements Q32
- Three elements Q33

4-membered rings containing:
- One element Q41
- Two elements Q42
- Three elements Q43
- Four elements Q44

5-membered rings containing:
- One element Q51
- Two elements Q52
- Three elements Q53
- Four elements Q54
- Five elements Q55

6-membered rings containing:
- One element Q61
- Two elements Q62
- Three elements Q63
- Four elements Q64
- Five elements Q65
- Six elements Q66

7-membered rings containing:
- One element Q71
- Two elements Q72
- Three elements Q73
- Four elements Q74
- Five elements Q75
- Six elements Q76
- Seven elements Q77

8-membered rings containing:
- One element Q81
- Two elements Q82
- Three elements Q83
- Four elements Q84
- Five elements Q85
- Six elements Q86
- Seven elements Q87
- Eight elements Q88

9- or more-membered rings containing:
- One element Q91
- Two elements Q92
- Three elements Q93
- Four elements Q94
- Five elements Q95
- Six elements Q96
- Seven elements Q97
- Eight elements Q98
- Nine or more elements Q99

Unspecified ring containing no carbon . . QZZ

CENTRAL ATOMS - FAMILY R-- or T--*

A (Argon)
- A chain. . . . 00
- A° 07

Ac (Actinium)
- Ac chain . . . 0(12)
- Ac^{+3} 0E
- Ac° 0H

Ag (Silver)
- Ag chain . . . 0(11)
- Ag^{+3} 0M
- Ag^{+2} 0N
- Ag^{+1} 0Ø
- Ag° 0P

Al (Aluminum)
- Al chain . . . 10
- Al^{+3} 12
- Al° 15

Am (Americium)
- Am chain . . 1(12)
- Am^{+3} 1E
- Am° 1H

As (Arsenic)
- As chain . . . 1(11)
- As^{+5} 1J
- As^{+4} 1K
- As^{+3} 1L
- As^{+2} 1M
- As° 1Ø
- As^{-3} 1R

At (Astatine)
- At chain . . . 20
- At° 28

Au (Gold)
- Au chain . . . 2(12)
- Au^{+3} 2D
- Au^{+2} 2E
- Au^{+1} 2F
- Au° 2G

B (Boron)
- B chain . . . 2(11)
- B^{+3} 2K
- B° 2N
- B^{-3} 2Q

Ba (Barium)
- Ba chain . . . 30
- Ba^{+2} 35
- Ba° 37

Be (Beryllium)
- Be chain . . . 3(12)
- Be^{+2} 3E
- Be° 3G

Bi (Bismuth)
- Bi chain . . . 3(11)
- Bi^{+5} 3J
- Bi^{+4} 3K
- Bi^{+3} 3L
- Bi^{+2} 3M
- Bi° 3Ø
- Bi^{-3} 3R

Br (Bromine)
- Br chain . . . 40
- Br^{+7} 41
- Br^{+5} 43
- Br^{+3} 45
- Br^{+1} 47
- Br° 48
- Br^{-1} 49

C (Carbon)
- C chain. . . . 4(12)
- C^{+4} 4A
- C^{+2} 4C
- C° 4E
- C^{-2} 4G
- C^{-4} 4I

Ca (Calcium)
- Ca chain . . . 4(11)
- Ca^{+2} 4N
- Ca° 4P

Cb (Columbium)
- Cb chain . . . 50
- Cb^{+5} 51
- Cb^{+4} 52
- Cb^{+3} 53
- Cb^{+2} 54
- Cb° 56

Cd (Cadmium)
- Cd chain . . . 5(12)
- Cd^{+2} 5E
- Cd° 5G

Ce (Cerium)
- Ce chain . . . 5(11)
- Ce^{+4} 5K
- Ce^{+3} 5L
- Ce° 5Ø

Cl (Chlorine)
- Cl chain . . . 60
- Cl^{+7} 61
- Cl^{+5} 63
- Cl^{+4} 64
- Cl^{+3} 65
- Cl^{+2} 66
- Cl^{+1} 67
- Cl° 68
- Cl^{-1} 69

Cm (Curium)
- Cm chain . . 6(12)
- Cm^{+3}. 6E
- Cm° 6H

Co (Cobalt)
- Co chain . . . 6(11)
- Co^{+4} 6N
- Co^{+3} 6Ø
- Co^{+2} 6P
- Co° 6R

Cr (Chromium)
- Cr chain . . . 70
- Cr^{+6} 72
- Cr^{+4} 74
- Cr^{+3} 75
- Cr^{+2} 76
- Cr^{+1} 77
- Cr° 78

Cs (Cesium)
- Cs chain . . . 7(12)
- Cs^{+1} 7F
- Cs° 7G

Cu (Copper)
- Cu chain . . . 7(11)
- Cu^{+3} 7M
- Cu^{+2} 7N
- Cu^{+1} 7Ø
- Cu° 7P

Dy (Dysprosium)
- Dy chain . . . 80
- Dy^{+3} 83
- Dy° 86

Er (Erbium)
- Er chain . . . 8(12)
- Er^{+3} 8C
- Er° 8F

Eu (Europium)
- Eu chain . . . 8(11)
- Eu^{+3} 8L
- Eu^{+2} 8M
- Eu° 8Ø

F (Fluorine)
- F chain. . . . 90
- F^{+7}. 91
- F^{+5}. 93
- F^{+3}. 95
- F^{+1}. 97
- F° 98
- F^{-1}. 99

* Superscript (°) signifies zero or indeterminate oxidation state.

CENTRAL ATOMS - FAMILY R-- or T--

Fa (Francium)
- Fa chain . . . 9(12)
- Fa^{+1} 9F
- Fa° 9G

Fe (Iron)
- Fe chain . . . 9(11)
- Fe^{+6} 9L
- Fe^{+4} 9N
- Fe^{+3} 9Ø
- Fe^{+2} 9P
- Fe° 9R

Ga (Gallium)
- Ga chain . . . A0
- Ga^{+3} A2
- Ga^{+2} A3
- Ga° A5

Gd (Gadolinium)
- Gd chain . . . A(12)
- Gd^{+3} . . . . . AC
- Gd° . . . . . AF

Ge (Germanium)
- Ge chain . . . A(11)
- Ge^{+4} . . . . . AJ
- Ge^{+2} . . . . . AL
- Ge° . . . . . AN
- Ge^{-2} . . . . . AP
- Ge^{-4} . . . . . AR

H (Hydrogen)
- H chain . . . B0
- H^{+1} B6
- H° B7
- H^{-1} B8

He (Helium)
- He chain . . . B(12)
- He° . . . . . BG

Hf (Hafnium)
- Hf chain . . . B(11)
- Hf^{+4} . . . . . BJ
- Hf° . . . . . BN

Hg (Mercury)
- Hg chain . . . C0
- Hg^{+2} C5
- Hg^{+1} C6
- Hg° C7

Ho (Holmium)
- Ho chain . . . C(12)
- Ho^{+3} CC
- Ho° . . . . . CF

I (Iodine)
- I chain . . . . C(11)
- I^{+7} . . . . . CJ
- I^{+5} CL
- I^{+3} . . . . . CN
- I^{+1} . . . . . CP
- I° . . . . . CQ
- I^{-1} . . . . . CR

In (Indium)
- In chain . . . D0
- In^{+3} D2
- In° D5

Ir (Iridium)
- Ir chain . . . D(12)
- Ir^{+6} . . . . . DC
- Ir^{+4} . . . . . DE
- Ir^{+3} . . . . . DF
- Ir^{+2} . . . . . DG
- Ir° . . . . . DI

K (Potassium)
- K chain . . . D(11)
- K^{+1} . . . . . DØ
- K° . . . . . DP

Kr (Krypton)
- Kr chain . . . E0
- Kr° E7

La (Lanthanum)
- La chain . . . E(12)
- La^{+3} . . . . . EC
- La° . . . . . EF

Li (Lithium)
- Li chain . . . E(11)
- Li^{+1} . . . . . EØ
- Li° . . . . . EP

Lu (Lutetium)
- Lu chain . . . F0
- Lu^{+3} F3
- Lu° F6

Mg (Magnesium)
- Mg chain . . . F(12)
- Mg^{+2} . . . . . FE
- Mg° . . . . . FG

Mn (Manganese)
- Mn chain . . . F(11)
- Mn^{+7} . . . . . FJ
- Mn^{+6} . . . . . FK
- Mn^{+4} . . . . . FM
- Mn^{+3} . . . . . FN
- Mn^{+2} . . . . . FØ
- Mn^{+1} . . . . . FP
- Mn° . . . . . FQ

Mo (Molybdenum)
- Mo chain . . . G0
- Mo^{+6} G2
- Mo^{+5} G3
- Mo^{+4} G4
- Mo^{+3} G5
- Mo^{+2} G6
- Mo° G8

N (Nitrogen)
- N chain . . . G(12)
- N^{+5} . . . . . GA
- N^{+4} . . . . . GB
- N^{+3} . . . . . GC
- N^{+2} . . . . . GD
- N^{+1} . . . . . GE
- N° . . . . . GF
- N^{-1} . . . . . GG
- N^{-2} . . . . . GH
- N^{-3} . . . . . GI

Na (Sodium)
- Na chain . . . G(11)
- Na^{+1} . . . . . GØ
- Na° . . . . . GP

Nd (Neodymium)
- Nd chain . . . H0
- Nd^{+3} H3
- Nd° H6

Ne (Neon)
- Ne chain . . . H(12)
- Ne° . . . . . HG

Ni (Nickel)
- Ni chain . . . H(11)
- Ni^{+6} . . . . . HL
- Ni^{+3} . . . . . HØ
- Ni^{+2} . . . . . HP
- Ni^{+1} . . . . . HQ
- Ni° . . . . . HR

Np (Neptunium)
- Np chain . . . I0
- Np^{+3} I5
- Np° I8

O (Oxygen)
- O chain . . . I(12)
- O° . . . . . IF
- O^{-2} . . . . . IH

Os (Osmium)
- Os chain . . . I(11)
- Os^{+8} . . . . . IJ
- Os^{+7} . . . . . IK
- Os^{+6} IL
- Os^{+4} . . . . . IN
- Os^{+3} . . . . . IØ
- Os° . . . . . IR

CENTRAL ATOMS - FAMILY R-- or T--

P (Phosphorus)
- P chain . . . J0
- P^{+5} J1
- P^{+4} J2
- P^{+3} J3
- P^{+2} J4
- P^{+1} J5
- P° J6
- P^{-1} J7
- P^{-2} J8
- P^{-3} J9

Pa (Protactinium)
- Pa chain . . . J(12)
- Pa^{+3} . . . . . JE
- Pa° . . . . . JH

Pb (Lead)
- Pb chain . . . J(11)
- Pb^{+4} . . . . . JJ
- Pb^{+2} . . . . . JL
- Pb° . . . . . JN

Pd (Palladium)
- Pd chain . . . K0
- Pd^{+4} K5
- Pd^{+2} K7
- Pd^{+1} K8
- Pd° K9

Pm (Promethium)
- Pm chain. . . V(11)
- Pm^{+3} VL
- Pm° . . . . . VØ

Po (Polonium)
- Po chain . . . K(12)
- Po° . . . . . KG

Pr (Praseodymium)
- Pr chain . . . K(11)
- Pr^{+3} . . . . . KL
- Pr° . . . . . KØ

Pt (Platinum)
- Pt chain . . . L0
- Pt^{+6} L3
- Pt^{+5} L4
- Pt^{+4} L5
- Pt^{+3} L6
- Pt^{+2} L7
- Pt° L9

Pu (Plutonium)
- Pu chain . . . L(12)
- Pu^{+6} . . . . . LB
- Pu^{+4} . . . . . LD
- Pu^{+3} . . . . . LE
- Pu° . . . . . LH

Ra (Radium)
- Ra chain . . . L(11)
- Ra^{+2} . . . . . LN
- Ra° . . . . . LP

Rb (Rubidium)
- Rb chain . . . M0
- Rb^{+1} M6
- Rb° M7

Re (Rhenium)
- Re chain . . . M(12)
- Re^{+7} . . . . . MA
- Re^{+6} . . . . . MB
- Re^{+5} . . . . . MC
- Re^{+4} . . . . . MD
- Re^{+3} . . . . . ME
- Re° . . . . . MH
- Re^{-1} . . . . . MI

Rh (Rhodium)
- Rh chain . . . M(11)
- Rh^{+6} . . . . . ML
- Rh^{+4} . . . . . MN
- Rh^{+3} . . . . . MØ
- Rh^{+2} . . . . . MP
- Rh° . . . . . MR

Rn (Radon)
- Rn chain . . . N0
- Rn° N7

Ru (Ruthenium)
- Ru chain . . . N(12)
- Ru^{+8} . . . . . NA
- Ru^{+7} . . . . . NB
- Ru^{+5} . . . . . ND
- Ru^{+4} . . . . . NE
- Ru^{+3} . . . . . NF
- Ru° . . . . . NI

S (Sulfur)
- S chain. . . . N(11)
- S^{+6} . . . . . NJ
- S^{+4} . . . . . NL
- S^{+2} . . . . . NN
- S° . . . . . NP
- S^{-2} . . . . . NR

Sb (Antimony)
- Sb chain . . . Ø0
- Sb^{+5} Ø1
- Sb^{+3} Ø3
- Sb° Ø6
- Sb^{-3} Ø9

Sc (Scandium)
- Sc chain . . . Ø(12)
- Sc^{+3} . . . . . ØC
- Sc° . . . . . ØF

Se (Selenium)
- Se chain . . . Ø(11)
- Se^{+6} . . . . . ØJ
- Se^{+4} . . . . . ØL
- Se^{+2} . . . . . ØN
- Se° . . . . . ØP
- Se^{-2} . . . . . ØR

Si (Silicon)
- Si chain . . . P0
- Si^{+4} P1
- Si° P5
- Si^{-2} P7
- Si^{-4} P9

Sm (Samarium)
- Sm chain. . . P(12)
- Sm^{+3} . . . . . PC
- Sm° . . . . . PF

Sn (Tin)
- Sn chain . . . P(11)
- Sn^{+4} . . . . . PJ
- Sn^{+2} . . . . . PL
- Sn° . . . . . PN
- Sn^{-4} . . . . . PR

Sr (Strontium)
- Sr chain . . . Q0
- Sr^{+2} Q5
- Sr° Q7

Ta (Tantalum)
- Ta chain . . . Q(12)
- Ta^{+5} . . . . . QA
- Ta^{+4} . . . . . QB
- Ta^{+3} . . . . . QC
- Ta° . . . . . QF

Tb (Terbium)
- Tb chain . . . Q(11)
- Tb^{+3} . . . . . QL
- Tb° . . . . . QØ

Tc (Technetium)
- Tc chain . . . R0
- Tc° R8

Te (Tellurium)
- Te chain . . . R(12)
- Te^{+6} . . . . . RA
- Te^{+4} . . . . . RC
- Te^{+2} . . . . . RE
- Te° . . . . . RG
- Te^{-2} . . . . . RI

Th (Thorium)
- Th chain . . . R(11)
- Th^{+4} . . . . . RM
- Th^{+3} . . . . . RN
- Th° . . . . . RQ

Ti (Titanium)
- Ti chain . . . S0
- Ti^{+4} S1
- Ti^{+3} S2
- Ti^{+1} S4
- Ti° S5

CENTRAL ATOMS - FAMILY R-- or T--

Tl (Thallium)
- Tl chain . . . S(12)
- Tl^{+3} . . . . . SB
- Tl^{+1} . . . . . SD
- Tl° . . . . . SE

Tm (Thulium)
- Tm chain . . S(11)
- Tm^{+3}. . . . . SL
- Tm° . . . . . SØ

U (Uranium)
- U chain . . . T0
- U^{+6}. T2
- U^{+4}. T4
- U^{+3}. T5
- U^{+2}. T6
- U^{+1}. T7
- U°. T8

V (Vanadium)
- V chain . . . T(12)
- V^{+5}. . . . . TA
- V^{+4}. . . . . TB
- V^{+3}. . . . . TC
- V^{+2}. . . . . TD
- V^{+1}. . . . . TE
- V°. . . . . TF

W (Tungsten)
- W chain . . . T(11)
- W^{+6} . . . . . TK
- W^{+5} . . . . . TL
- W^{+4} . . . . . TM
- W^{+3} . . . . . TN
- W^{+2} . . . . . TØ
- W° . . . . . TQ

Xe (Xenon)
- Xe chain . . . U0
- Xe°. U7

Y (Yttrium)
- Y chain. . . . U(12)
- Y^{+3}. . . . . UC
- Y°. . . . . UF

Yb (Ytterbium)
- Yb chain . . . U(11)
- Yb^{+3} . . . . . UL
- Yb^{+2} . . . . . UM
- Yb°. . . . . UØ

Zn (Zinc)
- Zn chain . . . V0
- Zn^{+2} V5
- Zn°. V7

Zr (Zirconium)
- Zr chain . . . V(12)
- Zr^{+4} . . . . . VA
- Zr°. . . . . VE

Unspecified cation or anion . ZZ

COORDINATE AND SOLVATE GROUPS - FAMILY S--, U-- or V-- *

Hydrogen

Hydrogen	H or H^+	01

Boron

Metaborates	HBO_2	11

Carbon

Alkynes	HC:CH	21
Alkenes	$H_2C:CH_2$	23
Alkanes or aromatic hydrocarbons	RH	25
Carbon monoxide	CO	28

Nitrogen

Ammonia	NH_3	31
Amido groups	$-NH_2$	32
Imido groups	-NH- (monodentate)	33
Imido groups	=NH (bidentate)	34
Nitrido groups	≡N	35
Amines, monoprimary	RNH_2 (monodentate)	3A
diprimary	$R(NH_2)_2$ (bidentate)	3B
polyprimary	$R(NH_2)_n$ (polydentate)	3C
monosecondary	RR'NH (monodentate)	3D
disecondary	$R(NHR')_2$ (bidentate)	3E
polysecondary	$R(NHR')_n$ (polydentate)	3F
monotertiary	RR'R"N (monodentate)	3G
ditertiary	$R(NR'R'')_2$ (bidentate)	3H
polytertiary	$R(NR'R'')_n$ (polydentate)	3I
Hydrazonium ions	$[NH_2NH_2H]^+$	3J
Hydrazines	$R_nN_2H_{4-n}$ (monodentate)	3L
	$R_nN_2H_{4-n}$ (bidentate)	3N
	NH_2NH_2	3P
Aminohydrazines	$RNHNHNH_2$	3R
Azides	$-N_3$	3S
Azo compounds	RN:NR'	3U
Guanidonium ions	$[NH_2C(:NH)NH_2H]^+$	3W
Guanidines	$NH_2C(:NH)NH_2$	3Y
Isocyanides	RNC	41
Nitriles	RCN	43
Cyanides	HCN	44
Metallo-cyanides	$H_xM_m(CN)_n$ (monodentate)	45
	$H_xM_m(CN)_n$ (bidentate)	46
	$H_xM_m(CN)_n$ (polydentate)	47
Cyanogen	$(CN)_2$	49

* In certain cases where R or M derivatives and the corresponding hydrogen derivatives are assigned separate code numbers, it is obvious that the H of the hydrogenated groups cannot be replaced by R or M. In all other cases, hydrogen may be replaced by R, by M or by the element to which the group is coordinated.

COORDINATE AND SOLVATE GROUPS - FAMILY S--, U-- or V--

Oxygen

Water	H_2O	61
Hydroxy groups	-OH	62
Oxo or oxy groups	(:O) or -O-	63
Peroxides	H_2O_2	65
	-OOH	66
	-OO-	67
Metal oxides	M_mO_n	68
Metallo-oxygen acid derivatives	$H_xM_mO_n$	69
Alcohols or phenols, mono-	ROH (monodentate)	6A
di-	$R(OH)_2$ (bidentate)	6B
poly-	$R(OH)_n$ (polydentate)	6D
Ethers, mono-	ROR' (monodentate)	6F
di-	$R(OR')_2$ (bidentate)	6G
poly-	$R(OR')_n$ (polydentate)	6I
Aldehydes	HC(:O)H	6J
Ketones, mono-	RR'C:O (monodentate)	6M
di-	$R(C:O)_2$ (bidentate)	6N
poly-	$R(C:O)_n$ (polydentate)	6P
Carbonates	HOC(:O)OH (monodentate)	6S
	HOC(:O)OH (bidentate)	6U
Carboxylates, mono-	HC(:O)OH (monodentate)	6V
di-	$R(C(:O)OH)_2$ (bidentate)	6X
poly-	$R(C(:O)OH)_n$ (polydentate)	6Y
Hydroxylamines	NH_2OH	71
Ureas	$NH_2C(:O)NH_2$	74
Amides	$HC(:O)NH_2$	78
Oximes, mono-	HC:NOH (monodentate)	7A
di-	$R(C:NOH)_2$ (bidentate)	7C
poly-	$R(C:NOH)_n$ (polydentate)	7E
Cyanates	HOCN	7J
Isocyanates	HNCO	7L
Nitrogen oxides	NO_2	7N
	NO	7Ø
Nitrosylo groups	$(NO)^-$	7S
Nitrosyl groups	$(NO)^+$	7T
Nitro groups	$-NO_2$	7V
Nitrites	-ONO	7W
Nitrates	$-ONO_2$	7X

Fluorine

Fluorine	F_2	91
Hydrogen fluoride derivatives	RF	92
	HF	93
	-F	94
Fluoro-oxygen acid derivatives	HFO_n	98

COORDINATE AND SOLVATE GROUPS - FAMILY S--, U-- or V--

Silicon

Metasilicates	H_2SiO_3 (monodentate)	BS
	H_2SiO_3 (bidentate)	BU

Phosphorus

Phosphines	PRR'R''	C1
	PHRR'	CA
	PH_2R	CD
	PH_3	CG
Phosphine oxides	PRR'R''O	CK
Phosphorus halides	PX_3	CM
	PX_5	CN
Phosphoryl halides	POX_3	CØ
Thiophosphoryl halides	PSX_3	CP
Metaphosphates	HPO_3	CS
Phosphates (ortho), organic	RH_2PO_4	CT
inorganic	H_3PO_4	CU
	$-H_2PO_4$	CV
	$=HPO_4$	CW
	$\equiv PO_4$	CX
Pyrophosphates	$H_4P_2O_7$	CY
Phosphites	H_2HPO_3	CZ

Sulfur

Hydrogen sulfide	H_2S	F1
Mercapto groups	-SH	F2
Thio groups	(:S) or -S-	F3
Di(or poly)sulfides	H_2S_n (n > 1)	F5
Thiols, mono-	RSH (monodentate)	FA
di(or poly)-	$R(SH)_n$ (bi(or poly)dentate)	FD
Thioethers, mono-	RSR' (monodentate)	FF
di-	$R(SR')_2$ (bidentate)	FG
poly-	$R(SR')_n$ (polydentate)	FI
Thiocarbonates	HSC(:S)SH	FS
	HSC(:S)OH or HSC(:O)SH	FT
	HSC(:O)OH or HOC(:S)OH	FU
Carbodithioates	HC(:S)SH	FV
Carbothioates	HC(:S)OH or HC(:O)SH	FW
Thiocyanates	HSCN	GJ
Isothiocyanates	HNCS	GL
Sulfur dioxide	SO_2	GN
Sulfur trioxide	SO_3	GØ
Sulfoxides	RR'SO	GS
Sulfones	$RR'SO_2$	GT
Thiosulfates	$H_2S_2O_3$ (monodentate)	GU
	$H_2S_2O_3$ (bidentate)	GV

COORDINATE AND SOLVATE GROUPS - FAMILY S--, U-- or V--

Sulfites, organic	$RHSO_3$	H1
inorganic	H_2SO_3	H2
	$-HSO_3$	H3
	$=SO_3$ (monodentate)	H4
	$=SO_3$ (bidentate)	H5
Sulfates, organic	$RHSO_4$	HA
inorganic	H_2SO_4	HB
	$-HSO_4$	HC
	$=SO_4$ (monodentate)	HD
	$=SO_4$ (bidentate)	HE
Sulfur halides	SX_n	HH

Chlorine

Chlorine	Cl_2	I1
Hydrogen chloride derivatives	RCl	I2
	HCl	I3
	-Cl	I4
Chloro-oxygen acid derivatives	$HClO_n$	I8

Arsenic

Arsines	AsH_3	LA
Arsenic halides	AsX_3	LM
Arsenic-oxygen acid derivatives	$H_xAs_mO_n$ (monodentate)	LS
	$H_xAs_mO_n$ (bi(or poly)dentate)	LU

Selenium

Hydrogen selenide	H_2Se	Ø1
Selenyl groups	-SeH	Ø2
Seleno groups	(:Se) or -Se-	Ø3
Di(or poly)selenides	H_2Se_n (n > 1)	Ø5
Selenols or selenoethers	RSeH	ØA
Seleno-oxygen acid derivatives	$H_xSe_mO_n$ (monodentate)	ØS
	$H_xSe_mO_n$ (bi(or poly)dentate)	ØU

Bromine

Bromine	Br_2	R1
Hydrogen bromide derivatives	RBr	R2
	HBr	R3
	-Br	R4
Bromo-oxygen acid derivatives	$HBrO_n$	R8

COORDINATE AND SOLVATE GROUPS - FAMILY S--, U-- or V--

Antimony

Stibines	SbH_3	TA
Antimony halides	SbX_3	TM
Antimony-oxygen acid derivatives	$H_xSb_mO_n$ (monodentate)	TS
	$H_xSb_mO_n$ (bi(or poly)dentate)	TU

Tellurium

Hydrogen telluride	H_2Te	W1
Telluryl groups	-TeH	W2
Telluro groups	(:Te) or -Te-	W3
Di(or poly)tellurides	H_2Te_n (n > 1)	W5
Tellurols or telluroethers	RTeH	WA
Telluro-oxygen acid derivatives	$H_xTe_mO_n$ (monodentate)	WS
	$H_xTe_mO_n$ (bi(or poly)dentate)	WU

Iodine

Iodine	I_2	Z1
Hydrogen iodide derivatives	RI	Z2
	HI	Z3
	-I	Z4
Iodo-oxygen acid derivatives	HIO_n	Z8

Specified groups

Coordinate or solvate groups which are not specifically designated in above table	ZW

Unspecified groups

Coordinate or solvate groups of indeterminate structure	ZZ

DIVISION IV - INDETERMINATE STRUCTURES

FAMILY Z--

In this family only the main headings are given. Further extension of subheadings may be made as occasion requires.

Proteins	Z10
Polypeptides	Z1A
Reaction products of proteins	Z20
Polysaccharides	Z30
Starch	Z35
Dextrins	Z3A
Cellulose	Z3K
Reaction products of polysaccharides	Z40
Lignins	Z50
Reaction products of lignins	Z60
Lipides	Z70
Reaction products of lipides	Z80
Other Natural Polymers	Z90
Gums	Z9A
Resins	Z9K
Rubbers	Z9S
Reaction products of other natural polymers	ZA0
Synthetic Polymers	ZB0
Resins	ZC0
Rubbers	ZD0
Reaction products of synthetic polymers	ZE0
Natural products of undetermined constitution not listed above	ZK0
Alkaloids	ZKA
Reaction products of carbon compounds of undetermined composition not already covered	ZS0
Unspecified heterocyclic structures containing carbon	ZZ0
Unspecified structures containing carbon	ZZA
Unspecified structures containing no carbon	ZZK
Indeterminate compounds	ZZZ

APPENDIX A

UTILIZATION OF THE CODE

The Chemical Code described in detail in the preceding pages has been devised for use in classifying, indexing and sorting chemicals according to specific predetermined characteristics. As the number of known compounds probably exceeds 500,000, it is evident that machine methods must be used to handle the available information on even a small fraction of the compounds. It is the purpose of this appendix to present the philosophy of the use of the code along with some elementary practical information about the equipment and its use including suggestions and illustrations on searching for compounds with selected characteristics.

The basic requirement of all machine methods is to mark or identify each characteristic or unit of the subjects at hand in such a way that mechanical methods can be employed in identifying and sorting the subjects according to the information desired. Several mechanical systems have been developed by various companies. The machines developed by both Remington Rand, Inc. and the International Business Machines Corporation are equally applicable to this type of coding. In the development of the chemical code, it has been convenient to utilize IBM equipment, and the description applies to that equipment.

The desired information is coded by use of letters and numbers as in the Chemical Code already described. This is translated into a form for mechanical handling by punching the appropriate combination of letters and numbers into designated areas on the special cards used in the machines. The cards are illustrated in Figs. 1 and 2.

A group of cards may be run through the machine, which contains a mechanism capable of sorting the cards into individual pockets as a result of electrical contacts made through the punched holes in the cards. While a single card of known punched characteristics could be selected from among many through a series of sorts on those unique characteristics punched on the card, it would not be a practical use of the machine. The value of the machine method lies in finding cards with certain selected characteristics from a large group. The machines will sort up to 24,000 cards per hour in a single column. No more information than is on the cards can be obtained, and the machines must be guided in the sorting. The machines relieve much of the repetitive physical effort involved in indexing and sorting, but the coding which precedes the card punching requires considerable time and technical knowledge. Actual operation of the machines would likely be in the hands of a technician unacquainted with chemistry. Accordingly, most efficient use of the code and mechanical sorting requires supervision by someone with an elementary understanding of the machines and an appreciation of the design of the code for correlation purposes. It is hoped that the following discussion will provide some of the elements required. Further details may be obtained from pamphlets published by the machine companies.

The Card. The card (3 1/4" x 7 3/8") upon which the data are recorded is of the type shown in Fig. 1. It contains spaces for punches in 80 columns with numbers from 0 to 9 in each column. In addition, there is an unmarked space above each column for two more punches. These are known as the 12 and 11 punches and are punched in Fig. 2. Combinations of the 12, 11 or 0 punch with the various numbers from 1 to 9 in any one column are used to designate the letters of the alphabet. Fig. 2 shows the punching of the letters. Each column therefore can provide any one of the 12 number or 26 letter designations. All cards must be sorted twice to pick out those cards punched with a particular letter in any one column. Only one of the 38 designations is possible in each column. If a larger number of possibilities is required, then two or more adjacent columns may be used. For example, three columns are used in describing the chemical groups (See List of Group Numbers, p. 29). This method of coding is called the field system. In contrast to this type of coding, a definite meaning may be assigned to each punch on the card. Such a procedure is termed direct coding and in the chemical code is employed in the coding of the families present and the empirical formula.

CARD LAYOUT

Column Numbers — **Significance of Columns**

1-6 — **Serial Number (000,001-999,999)**

7-9 — **Families Present**

Punch	Column 7	Column 8	Column 9
12	A	M	
11	B	N	Z
0	C	Ø	0
1	D	P	1
2	E	Q	2
3	F	R	3
4	G	S	4
5	H	T	5
6	I	U	6
7	J	V	7
8	K		8
9	L		9

10-49 — **Code of Chemical Structure**

10-13 — First "field" of four columns containing the group number for lowest numbered structural group. The four columns are punched according to Sec. 4.8: column 10, family designation, e.g., "1" in Fig. 4; columns 11 and 12, specific structure within the family, e.g., "77"; column 13, number of such groups (coded in previous three columns) in compound, e.g., "1". The entry in the first field in Fig. 4 is 1771.

14-49 — The next nine fields contain the remainder of the groups in ascending numeric and alphabetic order. If a compound contains more than 10 groups, the 11 punch in column 49 is used to indicate the presence of additional groups. A compound with more than 10 groups is not frequently encountered.

50-63 — **Empirical Formula**

50-55

Punch	Number of Atoms Column 50 + 51	52	53	54	55
12	C **	Br 1	F 1	N 1	O **
11		2	2	2	
0	0	3	3	3	
1	1	4	4	4	1
2	↓	5	5	5	2
3		6*	6*	6*	3
4		Cl 1	I 1	S 1	4
5		2	2	2	5
6		3	3	3	6
7		4	4	4	7
8		5	5	5	8
9	9 9#	6*	6*	6*	9***

* 6 or more or unspecified
** Unspecified
*** 9 or more
# 99 or more

CARD LAYOUT (cont.)

Column Numbers	Significance of Columns
50-63	
56-63	Presence of Other Elements Indicated

Punch	Column							
	56	57	58	59	60	61	62	63
12	A	Ca	Fa	K	Np	Re	Tb	Yb
11	Ac	Cb	Fe	Kr	Os	Rh	Tc	Zn
0	Ag	Cd	Ga	La	P	Rn	Te	Zr
1	Al	Ce	Gd	Li	Pa	Ru	Th	Pm
2	Am	Cm	Ge	Lu	Pb	Sb	Ti	
3	As	Co	H	Mg	Pd	Sc	Tl	
4	At	Cr	He	Mn	Po	Se	Tm	
5	Au	Cs	Hf	Mo	Pr	Si	U	
6	B	Cu	Hg	Na	Pt	Sm	V	
7	Ba	Dy	Ho	Nd	Pu	Sn	W	
8	Be	Er	In	Ne	Ra	Sr	Xe	
9	Bi	Eu	Ir	Ni	Rb	Ta	Y	

64-80 Physical or Biological Properties or Other Data

Fig. 3 shows the card layout diagramatically, and Figs. 4 to 8 show the actual punching for several types of compounds.

Use of the code may be facilitated by the preparation of as many cards as there are groups in the chemical code of a compound. By filing a card under each group present, all compounds containing a specific group may be selected with a minimum of effort. It is suggested that the code designations on the individual cards be so rotated that each group in turn appears in the first field (columns 10 to 13) of the card. When a compound contains more than ten groups, a second card should be made with the additional groups for filing purposes. Compounds containing two or more groups in common would be selected by matching in a collator (See p. 76) the serial numbers of the cards filed in the two desired groups. The serial number of the compound appears in columns 1 to 6 of all of the cards and is used for all collation processes.

The families present and the empirical formula are included as aids in sorting. It should be noted that the empirical formula is not a true empirical formula in that the number of atoms present is not shown in every case. The empirical formula is especially useful in locating all compounds containing a specific element or several atoms of the same element.

Columns 64 to 80 may be developed to suit the special problems of interest to the user.

The Machines. The key punch and sorter are basic equipment for a punched card installation. The punch is similar to a typewriter with a key for each number or letter. The printing punch prints the code at the top of the card as the characters are punched. The duplicating punch duplicates the cards by reproducing each column in order. The simple sorter sorts the cards into groups according to the punches in a single column. When sorting on the entire column, the punch which is at the lowest position in the column activates the sorting mechanism, i.e., the 9 punch takes precedence over a zero punch. For that reason, when one column contains letter punches, two sorts are necessary to select those cards with a specific letter. The sorter is equipped with a mechanism which blocks out any desired punches and allows sorting for any single punch as is necessary in the use of direct coding. For example, all compounds containing Family A-- may be separated by sorting in column 7 for the 12 punch. All cards which are not punched in this position will be rejected without disturbing the order. Likewise, all compounds containing mercury may be separated by sorting for punch 6 in column 58.

EXAMPLES INDEX

For large installations, several other machines may be used, which will simplify the location of the desired material. A multiple selector may be attached to the simple sorting machine. This allows the selection of any desired combination of numeric and/or alphabetic punches in any ten adjacent columns. This device can be used only when simple numeric or alphabetic punches are used and is not adaptable to direct coding. The reproducer reproduces the entire card in one process. The collator is especially useful for matching cards of one series with cards in another series. For example, by means of the serial number, a group of cards containing information on physical properties may be matched with a group containing information on biological properties. If all insecticidal compounds with a melting point of more than 100° C are desired, the cards from each group containing the desired property are arranged in serial number order and placed in the collator, which will then pick out all compounds possessing both of these properties. The interpreter interprets the cards after they have been punched by printing the code at the top of the card. The tabulator lists on a sheet of paper the code printed on a group of cards and is useful in comparing quickly the codes of groups of selected compounds.

Sorting Methods. Specific rules can not be given for the most rapid method of locating cards containing the desired characteristics. The method of answering a question will depend largely upon the type of question asked. Familiarity with the code and with the performance of the machines leads to the use of many short cuts in locating the desired information. Likewise, an organized assignment of serial number or the use of separate cards for each chemical group present decreases the number of cards which must be sorted to find any specific type of compound.

In the discussion below, it is assumed that only the sorter is available and that none of these special methods have been used. The location of all compounds containing the sulfonamide group (170, 171, 174 and 177) may be accomplished by sorting in the first field or column 10 for the 1 punch. All compounds which fall in the zero pocket must be saved to sort in column 14 for the presence or absence of Family 1--. The cards in pockets 2 to 9 may be rejected since these will contain no compounds with a group in Family 1--. The cards in the 1 pocket must be sorted to determine whether this is a numeric or alphabetic punch since A and J are a combination of the (12) (1) and (11) (1) punches, respectively. The cards with a 1 punch must then be sorted in column 11 for a 7 punch. The cards falling into the 0 to 6 pockets must be combined with the cards saved for sorting in column 14 and those in the 8 and 9 pockets may be discarded. Since alphabetic punches are not used in the second digit of Family 1--, it is not necessary to sort these cards again for alphabetic punching, and all of the cards in the 7 pocket are sulfonamides. The cards saved for sorting in column 14 may now be combined and treated in a similar fashion in columns 14 and 15. If any cards still fall in the zero pocket when sorted in column 14, they must be sorted in columns 18 and 19 in the same way. The multiple selector would shorten the sorting time by searching in two columns simultaneously.

Broad questions such as the location of all compounds containing a specific element can best be answered by sorting for the punch designating the presence of that element in the empirical formula.

The columns showing the families present were not used in the sort for the sulfonamide group because relatively few compounds would contain groups in Family 0--. If it is desired to locate all compounds containing a noncyclic disulfide group, it would be advisable to sort for the presence of Family J-- in column 7, punch 7 before sorting in column 10 to 49 for J63. Maintainence of separate files for each group present would eliminate sorting for a single specified group.

In many cases, it will be necessary to make the final sort by hand. For example, propyl esters can not be specifically located by the machines. A machine search locates all compounds containing both an ester of an aliphatic or alicyclic alcohol and C_3 saturated chain. The cards selected in this fashion must then be examined by hand and compared with the structure to determine whether or not a propyl ester is present. Likewise, in locating heterocyclic fused rings, hand sorting is necessary. For example, a benzothiazole ring is coded as a fused benzene ring and a C_3NS ring with maximum unsaturation. After all compounds containing these characteristics have been selected by machine, a hand sort and a comparison with the structure are necessary to determine whether or not the compound contains the benzothiazole ring. In general, experience will indicate the most expeditious method of locating the desired material.

Adequate definition of a question is essential to obtaining the desired answer with a minimum of sorting. Extreme care must be used in deciding which groups are to be searched for in order to answer a question properly. For example, in locating all urea derivatives the inclusiveness of the term derivatives must be defined. If thioureas are to be included, then it is necessary to sort for 825 ($H_2NC(:S)NH_2$) as well as 625 ($H_2NC(:O)NH_2$). Furthermore, the urea group is a

constituent part of larger groups such as guanylureas (610), diacylureas (623) and monoacylureas (624). Hence, the searcher must first determine how broad the definition of derivatives is to be before the groups which fulfill these conditions are selected.

Upon first glance, it might appear that in correlation studies sorting would be more rapid if all large groups were double coded to include code designations for their constituent parts as well as for the group as a whole. Consideration of such a procedure shows it to be impractical. For instance, in coding a diacylurea in this way it would be necessary to include code designations for monoacylurea, urea and an amide. It would not only add an unnecessarily large number of groups to the coding of each compound, but in this specific instance it would be impossible to sort for amides without obtaining all urea derivatives including monoacyl-, diacyl- and guanyl-ureas. In short, such a procedure would prove exceedingly cumbersome by overloading the small groups with more complex groups which often would not be desired in a search for the simpler derivatives.

It is recognized that for correlation purposes it may be advantageous to double code beyond the amount recommended in Sec. 5.223 of the Rules and Directions when a group has no code designation listed and must be broken into its constituent parts for coding. It may happen that in splitting a large group into its component parts and coding it as separate entities a characteristic chemical structure is obscured. To avoid this, any portion of a group which is not adequately described by following the prescribed rules may be double coded. The code is sufficiently flexible to permit the user to identify as many component structures as may seem desirable. In Sec. 5.223 the uncoded fragment of a large group is coded by using the smallest group (highest code number) which adequately describes the uncoded fragment. An alternate method, which may be followed equally well, uses the largest group (lowest code number) which describes the uncoded fragment or any portion of it regardless of the amount of double coding involved. Whatever method is used, it is essential to code always in a reproducible manner. If a user deviates from the method described in the Rules and Directions for Coding Compounds, he should do so consistently in order that he would always obtain the same code for a given compound. It may be desirable in certain instances to double code compounds that exist as tautomers. Some code numbers represent both tautomers; however for others it will be necessary to use several code numbers to represent both tautomeric structures.

Specific Codification or Additions to the Code. The Chemical Codification Panel recognizes that provision for expansion of the code should be made for constituent groups which may increase in importance and for others in which coding may have been overlooked or considered unnecessary. Some groups may be coded in a manner which, at first glance, would not appear most logical but the coding adopted represents an attempt for maximum efficiency.

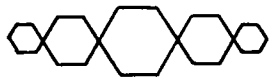
Certain groups may assume greater importance generally or may be more important for certain investigators. In that event, it may be desired to have a special punch for such groups if they are not already coded or coded only nonspecifically. While practical considerations forbid changes in the code numbers already assigned, the code can be expanded to include additional groups. Such expansion should be handled logically and uniformly in a manner consistent with the existing code. In the interest of uniformity, it is strongly suggested that any changes or additions be referred to the Chemical Codification Panel of the NRC Chemical-Biological Coordination Center. This would insure additions being made in a manner most in harmony with the concepts followed in development of the code.

If any user were interested in his own serial numbers and anticipated coding no more than 10,000 compounds, two columns of those used to designate the serial number could be saved for other uses. Even by using four columns for the serial number, the number handled could be increased to 30,000 by use of the 11 and 12 punches to designate successively the second and third 10,000 groups. Other 11 and 12 punches above the serial numbers or in certain other columns might be used to indicate sources of the compounds or to code certain bits of information. It should be pointed out that if collation on the serial number is contemplated, the use of the 11 and 12 punches should be restricted.

For those working in a special field such as arsenic or selenium chemistry, the empirical formula may be adapted to suit their purposes by assigning one or more columns to enumerate atoms of specific elements. The empirical formula as given is designated to cover the general field of organic and inorganic compounds.

Other examples of additions that might be suggested are a designation for the amide linkage of proteins and peptides. Investigators of steroids might wish special code numbers to describe more specifically certain aspects of the rings of the steroid nucleus.

Suggestions for expansion of the code have not been made to encourage modifications but with the understanding that some can be expected and that ways in which the code might be made more useful for the individual requirements should be suggested. It is hoped that the modifications in the main code will be minimum and that they can be made consistent with the rest of the code.



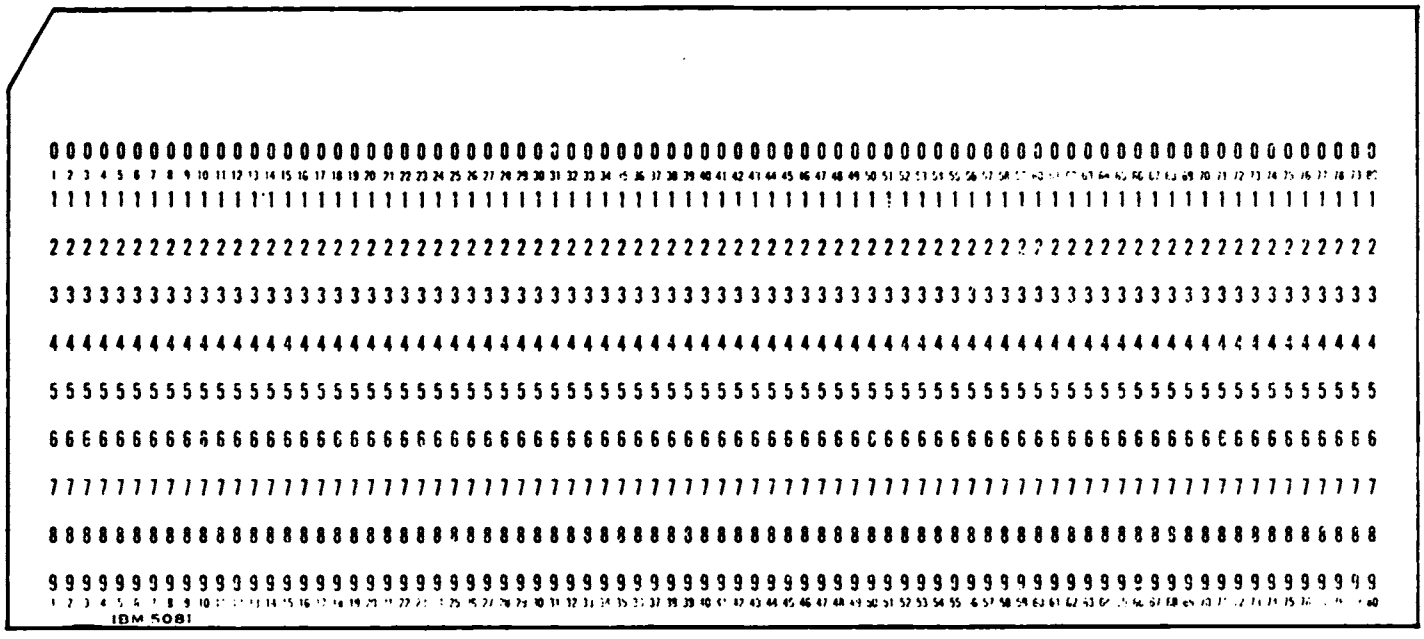


Fig. 1. The Card

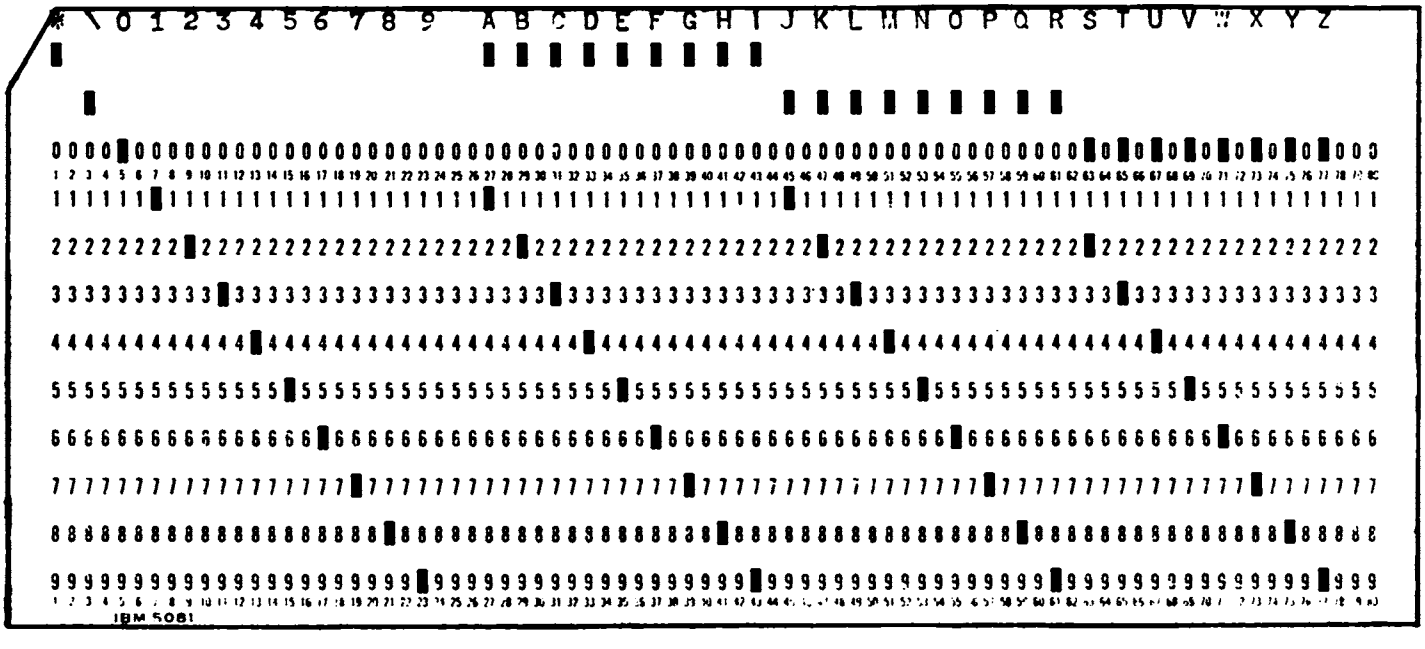


Fig. 2. Numeric and Alphabetic Punches

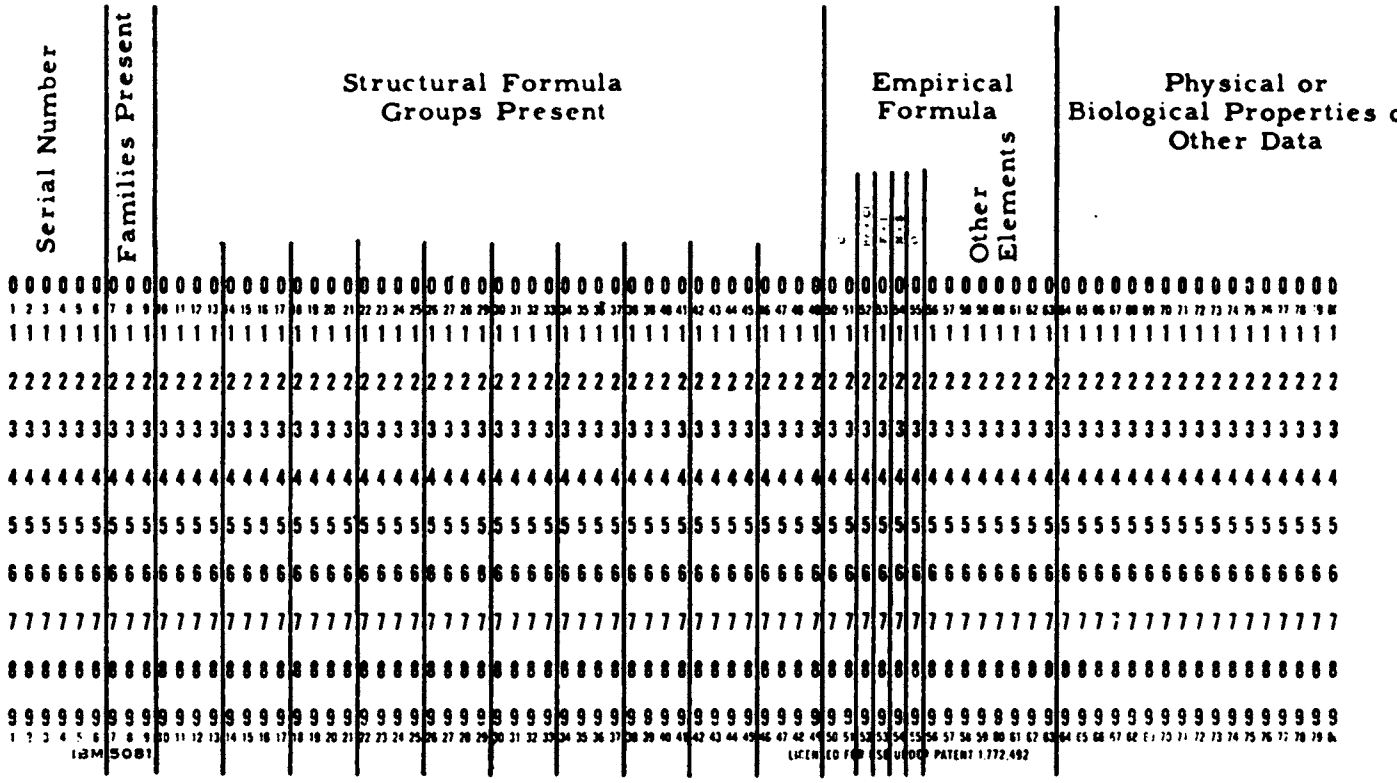


Fig. 3. Plan of Chemical Card

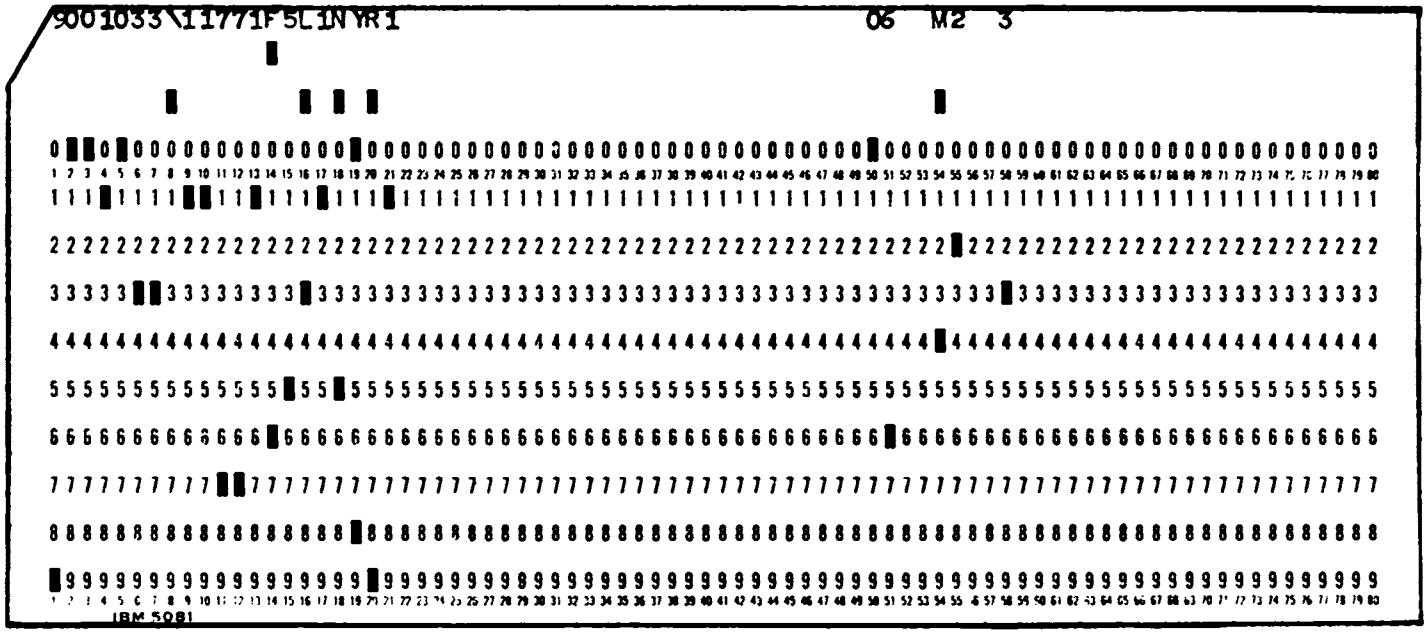
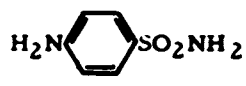


Fig. 4. Sulfanilamide $C_6H_8N_2O_2S$



177.1-F5L.1-NYR.1

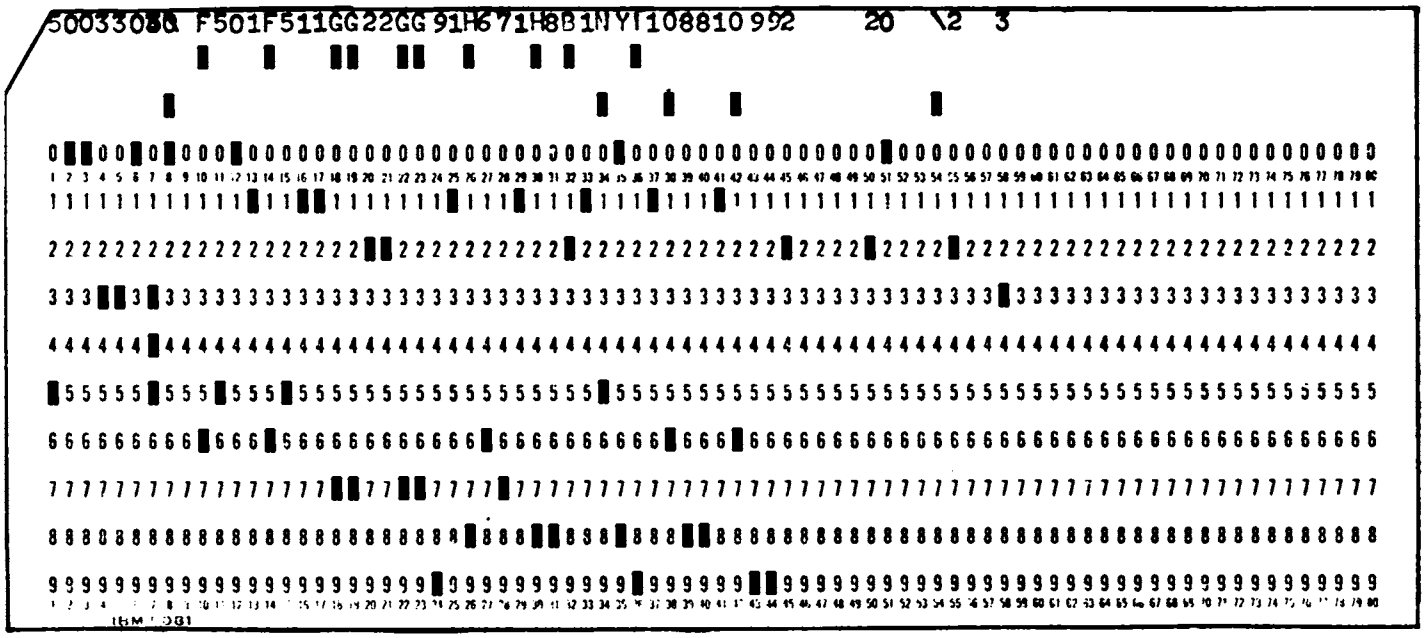
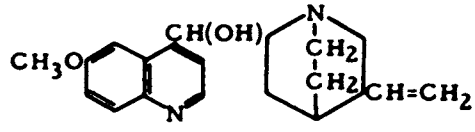


Fig. 5. Quinine $C_{20}H_{24}N_2O_2$



F50.1-F51.1-GG2.2-GG9.1-H67.1-H8B.1-NYI.1-ø88.1-ø99.2

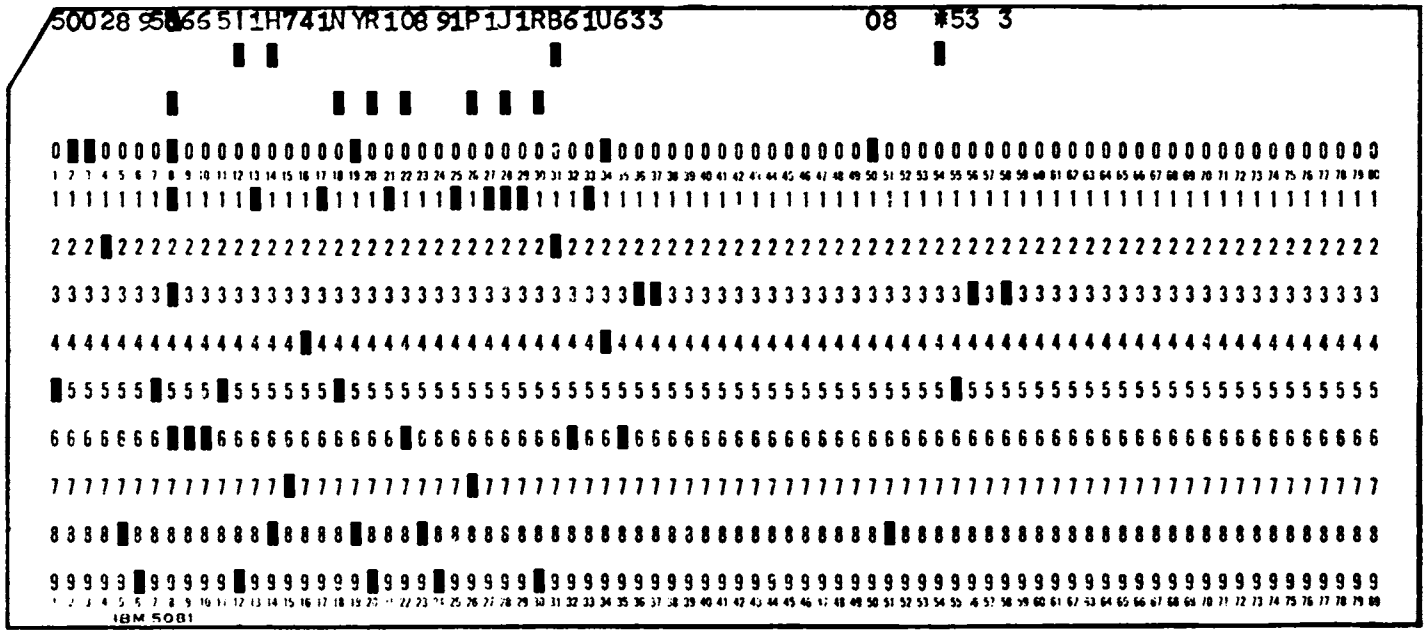
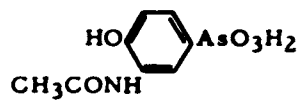


Fig. 6. Acetarsone $C_8H_{10}AsNO_5$



651.1-H74.1-NYR.1-ø89.1-PIJ.1-RB6.1-U63.3

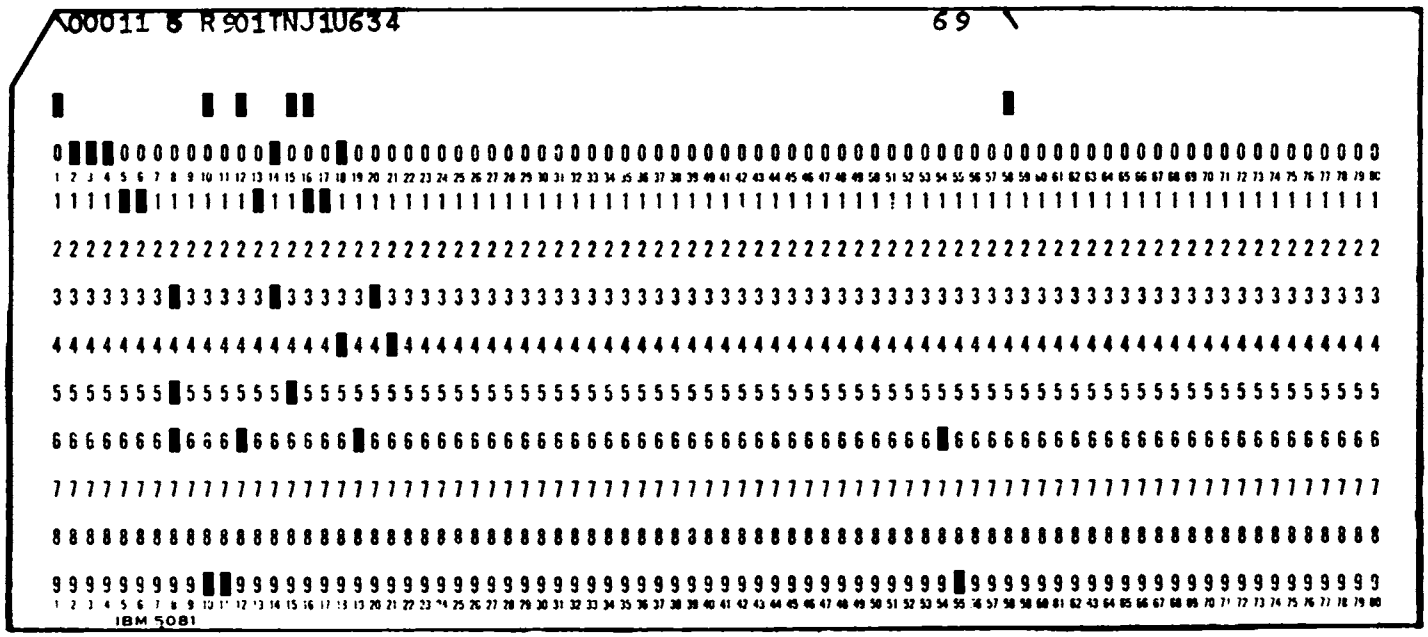


Fig. 7. Iron (III) sulfate $Fe_2O_{12}S_3$

$Fe_2(SO_4)_3$

R9Ø.1-TNJ.1-U63.4

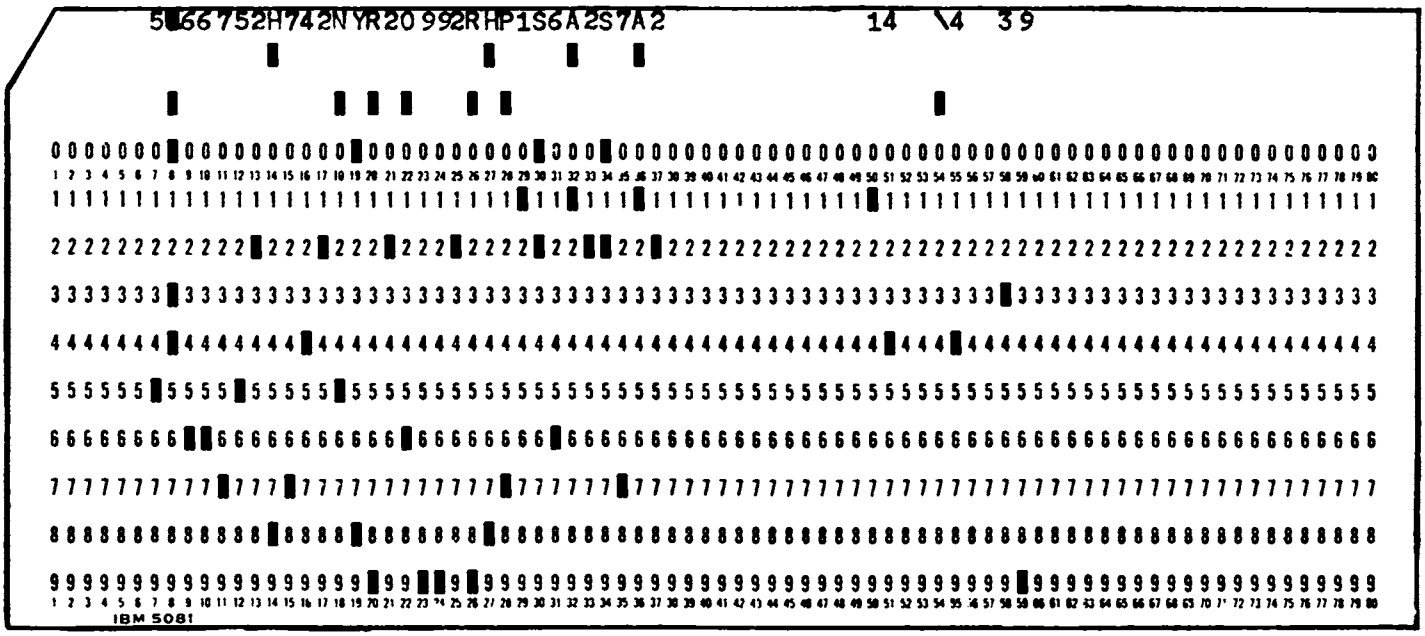
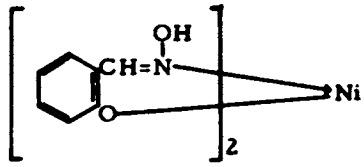


Fig. 8. Salicylaldehyde, oxime, nickel (II) complex $C_{14}H_{12}N_2NiO_4$



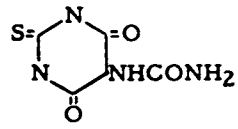
675.2-H74.2-NYR.2-Ø99.2-RHP.1-S6A.2-S7A.2

APPENDIX B

LIST OF EXAMPLES

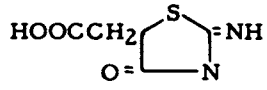
123.1-625.1-GFB.1-ø99.1

Pseudouric acid, 2-thio-



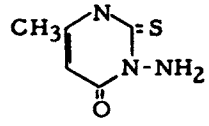
124.1-9ø2.1-H42.1-ø89.1

Thiazolidine-5-acetic acid, 2-imino-5-oxo-



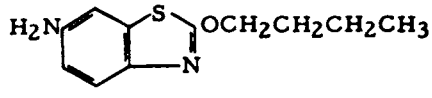
124.1-F35.1-GFC.1-ø99.1

Uracil, 3-amino-6-methyl-2-thio-



125.1-9ø9.1-F5L.1-NYI.1-ø7R.1

Benzothiazole, 6-amino-2-butoxy-



125.1-ø89.1-ø99.1

Carbamic acid, thiono-, ethyl ester

$H_2NC(:S)OC_2H_5$

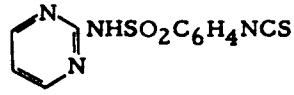
157.1-65C.1-F17.1-ø99.2

Ureasulfonic acid, guanyl-

$NH_2C(:NH)NHCONHSO_3H$

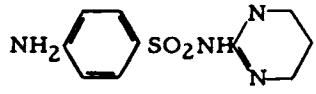
174.1-862.1-F50.2-GFI.1-NYR.1-ø99.1

Isothiocyanic acid, ester with p-(2-pyrimidylsulfamyl)phenol



174.1-F50.1-F5A.1-F5L.1-GFC.1-NYR.1

Sulfanilamide, N^1-(1,4,5,6-tetrahydro-2-pyrimidyl)-



174.1-F5L.1-H8I.1-L37.3-NYR.1-ø89.1-V61.2

Sulfanilamide, N^1-(2,2,2-trichloro-1-hydroxyethyl)-, sesquihydrate

$H_2NC_6H_4SO_2NHCH(OH)CCl_3 \cdot 1\text{-}1/2\ H_2O$

174.2-F5L.2-NYR.2-ø89.1

Sulfanilamide, N^1,N^1-ethylenedi-

$H_2NC_6H_4SO_2NHCH_2CH_2NHSO_2C_6H_4NH_2$

177.1-673.1-675.1-F5M.1-NYR.1-ø99.1

Benzamidoxime, p-(hydroxysulfamyl)-

$HONHO_2SC_6H_4C(:NOH)NH_2$

177.1-F5M.1-NYR.1-ø89.1-RB6.1-T69.1

Benzenesulfonamide, p-(2-aminoethyl)-, hydrochloride

$H_2NCH_2CH_2C_6H_4SO_2NH_2 \cdot HCl$

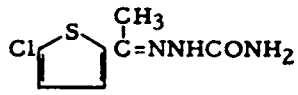
522.2-H67.2-NYR.2-ø89.1

Benzenesulfonyl chloride, p,p'-(ethylenedioxy)di-

$ClO_2SC_6H_4OCH_2CH_2OC_6H_4SO_2Cl$

620.1-J65.1-KP9.1-L32.1-ϕ89.1-ϕ99.1

Ketone, 5-chloro-2-thienyl methyl, semicarbazone



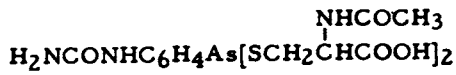
624.1-H32.1-ϕ89.1-ϕ99.1

Allophanic acid, ethyl ester

$H_2NCONHCOOC_2H_5$

625.1-65C.2-H42.2-NYR.1-ϕ7Z.2-ϕ89.2-ϕ99.1 P1L.1-UF3.2

Alanine, β,β'-(p-ureidophenylarsylenedithio)-bis[N-acetyl-



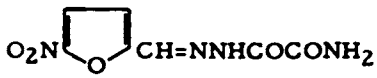
625.1-NYR.2-ϕ99.1-Pϕ1.2-RB6.1-U63.6

Benzenestibonic acid, p,p'-ureylenedi-

$H_2O_3SbC_6H_4NHCONHC_6H_4SbO_3H_2$

629.1-65L.1-685.1-H61.1-IP9.1-ϕ89.1-ϕ99.1

2-Furaldehyde, 5-nitro-, semioxamazone



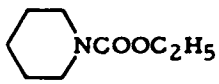
629.1-H32.2-ϕ89.2-ϕ99.2

Bicarbamic acid, diethyl ester

$C_2H_5OOCNHNHCOOC_2H_5$

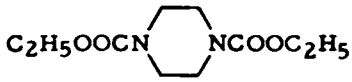
630.1-GH2.1-ϕ89.1-ϕ99.1

1-Piperidinecarboxylic acid, ethyl ester



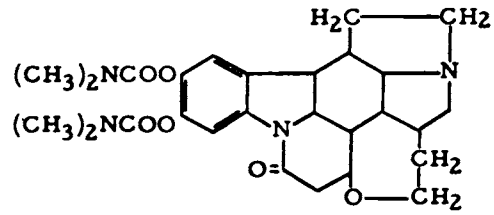
630.2-GFK.1-ϕ89.2-ϕ99.2

1,4-Piperazinedicarboxylic acid, diethyl ester



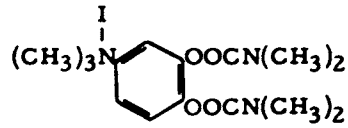
632.2-646.1-F51.1-GG2.2-GP2.1-GP5.1-H61.1-I9K.1-NYB.1-NYI.1-ϕ99.6

Bisapomethylbrucine, bis(dimethylcarbamate)



632.2-F46.1-NYR.1-ϕ99.9-TCR.1

Ammonium iodide, (3,4-dihydroxyphenyl)-trimethyl-, bis(dimethylcarbamate)



634.1-689.1-L37.1-ϕ7Z.1-ϕ99.2

Carbamic acid, (2-chloropropyl)nitroso-, methyl ester

$CH_3OOCN(NO)CH_2CHClCH_3$

634.1-F46.1-ϕ89.1-ϕ99.5-T69.1

Ammonium chloride, (2-hydroxyethyl)trimethyl-, methylcarbamate

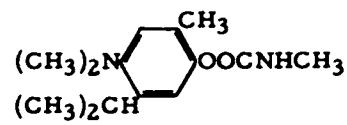
634.1-F57.1-H67.1-NYR.2-ϕ89.2-ϕ99.2

Carbanilic acid, p-methoxy-, m-diethylaminophenyl ester

$H_3COC_6H_4NHCOOC_6H_4N(C_2H_5)_2$

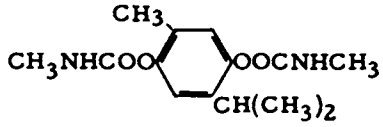
634.1-F57.1-NYR.1-ϕ7Z.1-ϕ99.5

Carbamic acid, methyl-, ester with 5-dimethylaminocarvacrol



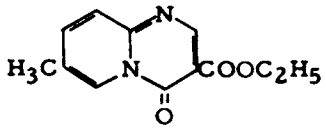
634.2-NYR.1-∅7Z.1-∅99.5

Carbamic acid, methyl-, diester with thymohydroquinone



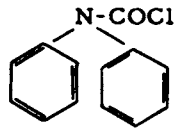
646.1-F50.1-GFD.1-GG4.1-H34.1-∅89.1-∅99.2

4H-Pyrido[1,2-a]pyrimidine-3-carboxylic acid, 4-oxo-7-methyl-, ethyl ester



652.1-D22.1-NYR.2-∅99.1

Carbamyl chloride, diphenyl-



65C.2-F5M.1-H42.1-∅7Z.1-∅89.2

Glycine, N-(N-alanylglycyl)-

$CH_3CH(NH_2)CONHCH_2CONHCH_2COOH$

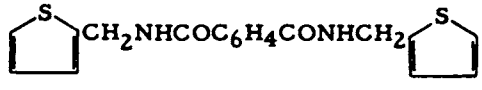
65C.4-F5M.1-H42.1-∅89.5

Glycine, N-{N-[N-(N-glycylglycyl)glycyl]-glycyl}-

$H_2NCH_2CO(NHCH_2CO)_3NHCH_2COOH$

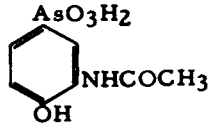
65G.2-J65.2-KP9.2-NYR.1-∅99.4

Phthalamide, N,N'-di(2-thenyl)-



65I.1-H74.1-NYR.1-∅89.1-P1J.1-RB6.1-U63.3

Acetarsone



65L.1-H42.1-∅7Q.1

Maleamic acid

$HOOCCH=CHCONH_2$

667.1-L37.2-∅89.2

Diethylamine, 2,2'-dichloro-N-nitroso-

$(ClCH_2CH_2)_2NNO$

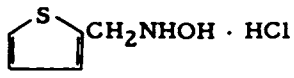
675.2-NYM.1

p-Quinone, dioxime

$HON=C_6H_4=NOH$

677.1-J65.1-KP9.1-∅99.1-RB6.1-T69.1

Hydroxylamine, N-(2-thenyl)-, hydrochloride



682.2-J63.1-NYR.2

Disulfide, bis(p-nitrophenyl)

$O_2NC_6H_4SSC_6H_4NO_2$

686.1-H5C.1-NYR.1-∅99.1

Benzaldehyde, p-nitro-

$O_2NC_6H_4CHO$

686.1-H8L.1-NYR.1-∅99.1

Benzyl alcohol, o-nitro-

$O_2NC_6H_4CH_2OH$

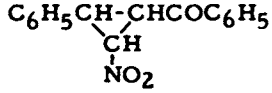
686.2-830.1-NYR.1-∅99.3

Carbamic acid, dimethyldithio-, 2,4-dinitrophenyl ester

$(CH_3)_2NCSSC_6H_3(NO_2)_2$

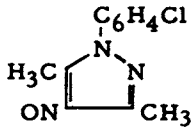
687.1-H57.1-NYR.2-NZK.1-∅99.1

Ketone, 2-nitro-3-phenylcyclopropyl phenyl



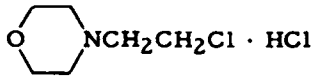
689.1-GN9.1-L35.1-NYR.1-ø99.2

Pyrazole, 1-(p-chlorophenyl)-3,5-dimethyl-4-nitroso-



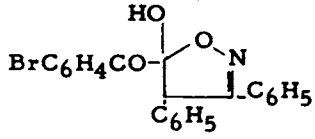
7I2.1-F51.1-H61.1-L37.1-ø89.1-RB6.1-T69.1

Morpholine, 4-(2-chloroethyl)-, hydrochloride



7ø5.1-H4M.1-H55.1-L45.1-NYR.3-ø99.1

Ketone, p-bromophenyl 5-hydroxy-3,4-diphenyl-2-isoxazolin-5-yl



805.1-ø99.6

Disulfide, bis(dimethylthiocarbamyl)

$(CH_3)_2NC(:S)SSC(:S)N(CH_3)_2$

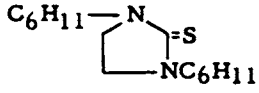
808.1-ø99.6

Sulfide, bis(dimethylthiocarbamyl)

$(CH_3)_2NC(:S)SC(:S)N(CH_3)_2$

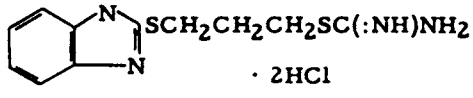
825.1-GN2.1-NYK.2

2-Imidazolidinethione, 1,3-dicyclohexyl-



825.2-GN9.1-NYI.1-ø7Z.1-ø99.1-RB6.1-T69.1

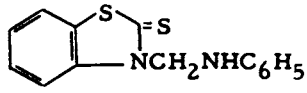
Benzimidazole, 2-(3-guanylmercaptopropyl)-mercapto-, dihydrochloride



· 2HCl

830.1-9ø5.1-F5G.1-NYI.1-NYR.1-ø99.1

2(3H)-Benzothiazolethione, 3-anilinomethyl-



A42.1-F46.1-F5L.1-H8M.1-NYR.1-ø89.1-ø99.3

Ammonium sulfanilate, (2-hydroxyethyl)-trimethyl-

$H_2NC_6H_4SO_3N(CH_3)_3CH_2CH_2OH$

A64.1-L27.2-ø89.2

Sulfuric acid, bis(2-fluoroethyl) ester

$(FCH_2CH_2O)_2SO_2$

A70.1-H74.2-NYR.2

Phenol, p,p'-sulfonyldi-

$HOC_6H_4SO_2C_6H_4OH$

A70.1-L37.1-ø88.1-ø89.1

Sulfone, 2-chloroethyl vinyl

$ClCH_2CH_2SO_2CH{=}CH_2$

A70.1-ø89.2-P1L.2-UI4.4

Sulfone, bis(2-dichloroarsinoethyl)

$(Cl_2AsCH_2CH_2)_2SO_2$

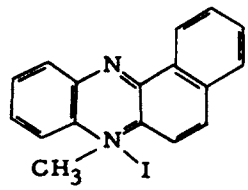
D40.1-NYR.1

Benzene, iodoso-

C_6H_5IO

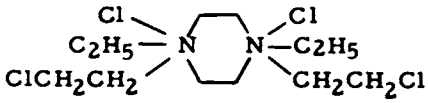
F41.1-F50.1-GFR.1-NTR.1-NYI.1-ø99.1-TCR.1

Benzo[a]phenazinium iodide, 7-methyl-



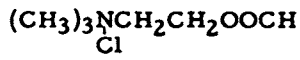
F43.2-GFK.1-L37.2-ø89.4-T69.1

Piperazinium dichloride, 1,4-bis(2-chloroethyl)-1,4-diethyl-



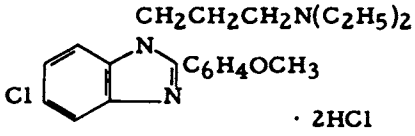
F46.1-H32.1-ø89.1-ø99.4-T69.1

Choline chloride, formate



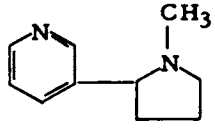
F50.1-F51.1-F54.1-GN9.1-H67.1-L35.1-NYI.1-NYR.1-ø7Z.1-ø89.2-ø99.1-RB6.1-T69.1

Benzimidazole, 5-chloro-1-(3-diethylaminopropyl)-2-(o-methoxyphenyl)-, dihydrochloride



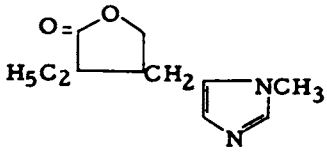
F50.1-F51.1-GH9.1-GP2.1-ø99.1

Nicotine



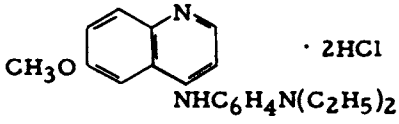
F50.1-F51.1-GN9.1-H26.1-IP2.1-ø89.1-ø99.2-RB6.1-T69.1

Pilocarpine, monohydrochloride



F50.1-F57.1-F5E.1-GG9.1-H67.1-NYI.1-NYR.1-ø89.2-ø99.1-RB6.1-T69.1

Quinoline, 4-(p-diethylaminoanilino)-6-methoxy-, dihydrochloride

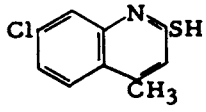


F50.1-F5F.1-GH9.1-H42.1-ø7Y.1-ø99.1

Acrylic acid, β-(5-methyl-2-pyridylamino)-

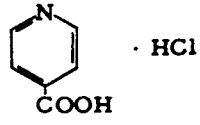
F50.1-GG9.1-J72.1-L35.1-NYI.1-ø99.1

Carbostyril, 7-chloro-4-methylthio-



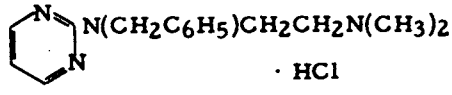
F50.1-GH9.1-H40.1-ø99.1-RB6.1-T69.1

Isonicotinic acid, hydrochloride



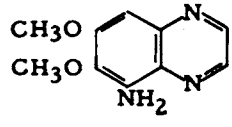
F50.2-F54.1-F56.1-GFI.1-NYR.1-ø89.1-ø99.3-RB6.1-T69.1

Pyrimidine, 2-[benzyl(2-dimethylaminoethyl)-amino]-, hydrochloride



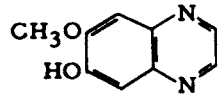
F50.2-F5L.1-GFR.1-H67.2-NYI.1-ø99.2

Quinoxaline, 5-amino-6,7-dimethoxy-



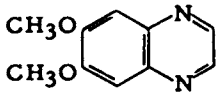
F50.2-GFR.1-H67.1-H74.1-NYI.1-ø99.1

6-Quinoxalinol, 7-methoxy-



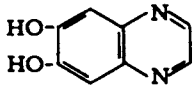
F50.2-GFR.1-H67.2-NYI.1-ø99.2

Quinoxaline, 6,7-dimethoxy-



F50.2-GFR.1-H74.2-NYI.1-RB6.1-T69.1

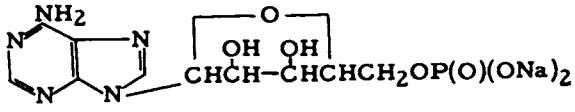
6,7-Quinoxalinediol, monohydrochloride



HCl

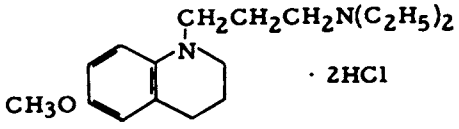
F50.3-F51.1-F5K.1-GFI.1-GN9.1-H61.1-H8A.2-IP2.1-ø99.1-RGø.1-TJ1.1-U63.4

Adenosine-5-phosphoric acid, disodium salt



F51.1-F54.1-GG3.1-H67.1-NYI.1-ø7Z.1-ø89.2-ø99.1-RB6.1-T69.1

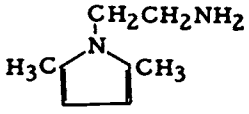
Quinoline, 1-(3-diethylaminopropyl)-1,2,3,4-tetrahydro-6-methoxy-, dihydrochloride



· 2HCl

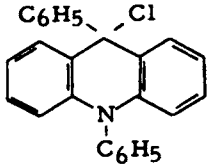
F51.1-F5M.1-GP9.1-ø89.1-ø99.2

Pyrrole, 1-(2-aminoethyl)-2,5-dimethyl-



F51.1-GG4.1-L32.1-NYI.2-NYR.2-RB6.1-T69.1

Acridan, 9-chloro-9,10-diphenyl-, hydrochloride



· HCl

F51.1-GH2.1-L37.1-ø89.1

Piperidine, 1-(2-chloroethyl)-

$C_5H_{10}NCH_2CH_2Cl$

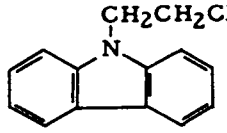
F51.1-GH2.1-L37.1-ø89.1-RB6.1-T69.1

Piperidine, 1-(2-chloroethyl)-, hydrochloride

$C_5H_{10}NCH_2CH_2Cl \cdot HCl$

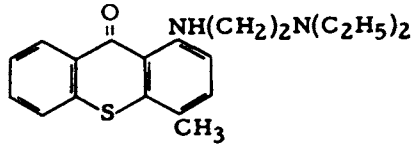
F51.1-GP9.1-L37.1-NYI.2-ø89.1

Carbazole, 9-(2-chloroethyl)-



F54.1-F5G.1-H51.1-J65.1-KH9.1-NYI.2-ø89.3-ø99.1

Thiaxanthone, 1-(2-diethylaminoethylamino)-4-methyl-



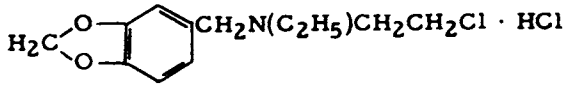
F54.1-H32.2-ø89.4-ø99.1

Ethanol, 2,2'-methyliminodi-, diacetate

$(CH_3COOCH_2CH_2)_2NCH_3$

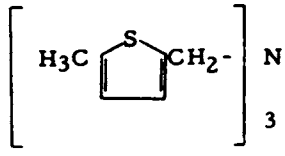
F54.1-H4J.1-IN9.1-L37.1-NYI.1-ø89.2-ø99.1 RB6.1-T69.1

Piperonylamine, N-2-chloroethyl-N-ethyl-, hydrochloride



F54.1-J65.3-KP9.3-ø99.6

Tri-2-thenylamine, 5,5',5''-trimethyl-



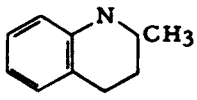
F57.1-F5L.1-NYR.1-ø99.2

p-Phenylenediamine, N,N-dimethyl-

$H_2NC_6H_4N(CH_3)_2$

F5A.1-GG3.1-NYI.1-ø99.1

Quinaldine, 1,2,3,4-tetrahydro-



F5D.1-L37.2-ø89.2-T2K.1-U94.3

Diethylamine, 2,2'-dichloro-, complex with 1 f. wt. boron trifluoride

$(ClCH_2CH_2)_2NH \cdot BF_3$

F5L.2-J63.1-NYR.2-RB6.1-T69.1

Aniline, p,p'-dithiodi-, dihydrochloride

$H_2NC_6H_4SSC_6H_4NH_2 \cdot 2HCl$

F5L.2-NYR.2-ø99.1

Aniline, p,p'-methylenedi-

$H_2NC_6H_4CH_2C_6H_4NH_2$

F5L.3-NYR.1-RB6.1-T69.1

1,3,5-Benzenetriamine, trihydrochloride

$C_6H_3(NH_2)_3 \cdot 3HCl$

F75.1-H42.1-H57.1-L35.1-NYR.2-ø6Z.1

Hydrocinnamic acid, β-(p-chlorophenacyl)-α-cyano-

$ClC_6H_4COCH_2CH(C_6H_5)CH(CN)COOH$

F75.1-H54.1-NYR.1-ø7R.1

Acetoacetonitrile, α-phenyl-

$CH_3COCH(C_6H_5)CN$

F75.1-H57.2-NYR.5-ø69.1

Butyronitrile, γ-benzoyl-α-(α-phenacylbenzyl)-α,β-diphenyl-

$C_6H_5COCH_2CH(C_6H_5)C(CN)(C_6H_5)CH(C_6H_5)$
$C_6H_5COCH_2$

F75.1-H8D.1-L37.1-ø7Z.1

Lactonitrile, β-chloro-

$CH_2ClCH(OH)CN$

F75.1-ø7R.2-ø7Z.1-PJ1.1-U63.3

Ethanephosphonic acid, 2-cyano-, dibutyl ester

$NCCH_2CH_2P(=O)(OCH_2CH_2CH_2CH_3)_2$

F75.1-ø99.1

Hydrocyanic acid

HCN

F75.1-ø99.1-RGø.1

Sodium cyanide

NaCN

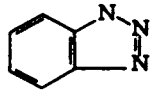
F75.6-ø99.6-RDø.1-T6P.1-U44.6

Potassium cyanocobaltate (II)

$K_4Co(CN)_6$

GL9.1-NYI.1

1H-Benzotriazole



H15.1-ø99.1-RGø.1

Sodium carbonate

$NaHCO_3$

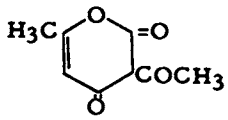
H15.1-ø99.1-RGø.1

Sodium carbonate

Na_2CO_3

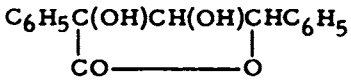
H26.1-H51.1-H56.1-IH5.1-ø89.1-ø99.1

Dehydroacetic acid



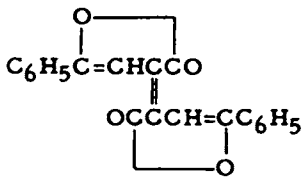
H26.1-H81.1-H8A.1-IP2.1-NYR.2

Butyric acid, α,β,γ-trihydroxy-α,γ-diphenyl-, γ-lactone



H26.2-IP5.2-NYR.2-ø08.1

Fumaric acid, bis(β-hydroxystyryl)-, dilactone



H32.1-H64.8-H8M.1-ø59.1-ø89.9

Lauric acid, monoester with nonaethylene glycol

$$HO(CH_2CH_2O)_8CH_2CH_2OOC(CH_2)_{10}CH_3$$

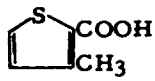
H32.2-L37.1-ø7Z.1-ø89.2

Malonic acid, chloro-, diethyl ester

$$ClCH(COOC_2H_5)_2$$

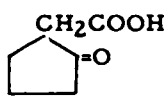
H40.1-J65.1-KP9.1-ø99.2

2-Thiophenecarboxylic acid, 3-methyl-



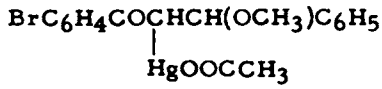
H42.1-H51.1-NZ2.1-ø89.1

Cyclopentaneacetic acid, 2-oxo-



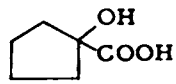
H42.1-H57.1-H64.1-L45.1-NYR.2-ø7Z.1-ø89.1-ø99.1-PC5.1-S6V.1

Propiophenone, α-acetoxymercuri-p-bromo-β-methoxy-β-phenyl-



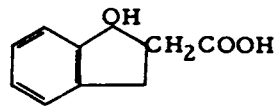
H42.1-H81.1-NZ2.1-ø99.1

Cyclopentanecarboxylic acid, 1-hydroxy-



H42.1-H8A.1-NVE.1-ø89.1

2-Indanacetic acid, 1-hydroxy-



H42.1-H8D.1-ø3Q.1-R35.1

Ricinoleic acid, barium salt

$$[CH_3(CH_2)_5CHOHCH_2CH{=}CH(CH_2)_7COO]_2Ba$$

H42.1-NYR.1-ø7Z.1-PC5.1-S6V.1

Mercury propionate, phenyl-

$$C_6H_5HgOOCCH_2CH_3$$

H42.1-ø5H.1-RV5.1

10-Hendecenoic acid, zinc salt

$$[CH_2{=}CH(CH_2)_8COO]_2Zn$$

H42.1-ø6I.1

Caproic acid, β-methyl-

$$CH_3(CH_2)_2CH(CH_3)CH_2COOH$$

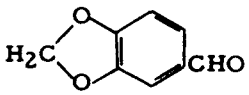
H42.2-L37.1-ø7Q.1

Fumaric acid, chloro-

$$HOOCCH{=}CClCOOH$$

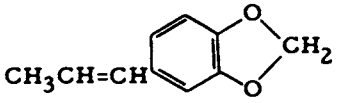
H4J.1-H5C.1-IN9.1-NYI.1-ø99.1

Piperonal



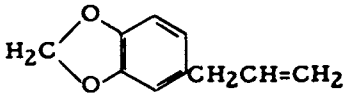
H4J.1-IN9.1-NYI.1-ø7Y.1

Isosafrole



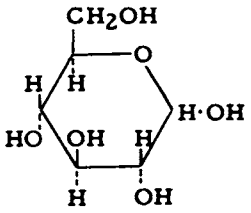
H4J.1-IN9.1-NYI.1-ø7Y.1

Safrole



H4M.1-H8A.3-H8K.1-IH2.1-ø99.1

D-Glucose



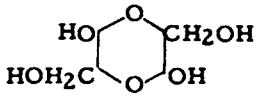
H4M.1-L35.1-L37.3-NYR.1-ø89.2

Chloral, p-chlorophenyl ethyl acetal

$ClC_6H_4OCH(CCl_3)OC_2H_5$

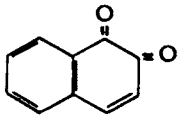
H4M.2-H8K.2-IF2.1-ø99.2

2,5-p-Dioxanedimethanol, 3,6-dihydroxy-



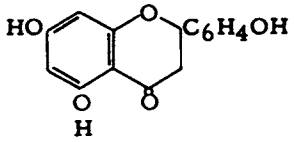
H50.1-NTø.1

1,2-Naphthoquinone



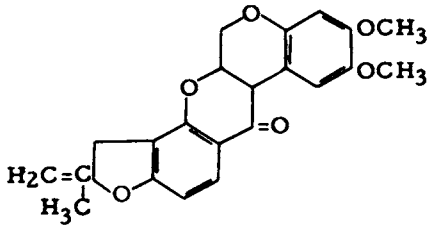
H51.1-H61.1-H74.3-IH5.1-NYI.1-NYR.1

Naringenin



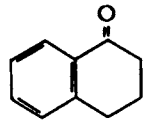
H51.1-H61.3-H67.2-IH5.2-IP5.1-NYI.2-ø7Y.1-ø99.2

Rotenone



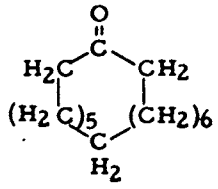
H51.1-NTN.1

1(2H)-Naphthalenone, 3,4-dihydro-



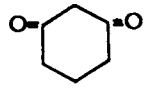
H51.1-NY2.1

Cyclopentadecanone



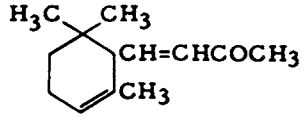
H51.2-NYK.1

1,3-Cyclohexanedione



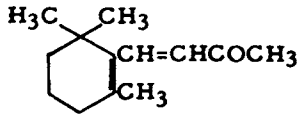
H54.1-NYL.1-ø7Q.1-ø99.3

α-Ionone



H54.1-NYL.1-ø7Q.1-ø99.3

β-Ionone



H57.1-L35.1-L45.1-NYR.2-ø7Y.1

Chalcone, 4'-bromo-4-chloro-

$ClC_6H_4CH{=}CHCOC_6H_4Br$

H5D.1-ø68.1

2-Hexenal, 2-ethyl-

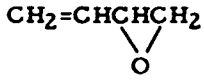
$CH_3CH_2CH_2CH{=}C(C_2H_5)CHO$

H61.1-IP2.1

Furan, tetrahydro-

H61.1-IX2.1-ø88.1

1-Butene, 3,4-epoxy-



H64.2-ø86.1-ø89.2-ø99.2-PC5.2

Mercury, ethynylenebis[2-methoxyethyl-

$CH_3OC_2H_4HgC{\equiv}CHgC_2H_4OCH_3$

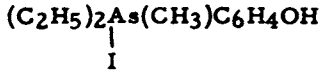
H67.1-H74.1-NYR.1-ø99.2

Creosol

$(CH_3O)(OH)C_6H_3CH_3$

H74.1-NYR.1-ø89.2-ø99.1-PlJ.1-TCR.1

Arsonium iodide, diethyl(3-hydroxyphenyl)-methyl-



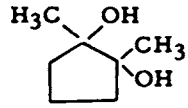
H74.2-NYR.1-ø99.1

4-Homopyrocatechol

$CH_3C_6H_3(OH)_2$

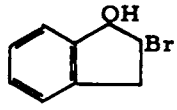
H81.2-NZ2.1-ø99.2

1,2-Cyclopentanediol, 1,2-dimethyl-



H8A.1-L47.1-NVE.1

1-Indanol, 2-bromo-



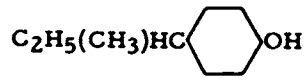
H8A.1-NYK.1

Cyclohexanol

$C_6H_{11}OH$

H8A.1-NYK.1-ø7R.1

Cyclohexanol, 4-sec-butyl-



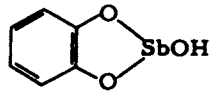
H8M.1-ø69.1

1-Hexanol, 2-ethyl-

$HOCH_2CH(C_2H_5)(CH_2)_3CH_3$

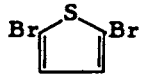
I2R.1-NYI.1-RB6.1-Tø3.1-U63.3

1,3,2-Benzodioxastibiole, 2-hydroxy-



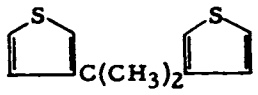
J65.1-KP9.1-L42.2

Thiophene, 2,5-dibromo-



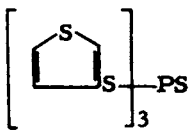
J65.1-KP9.2-ø7Z.1

Thiophene, 3,3'-isopropylidenedi-



J65.3-KP9.3-TJ1.1-UF3.4

3-Thienyl thiophosphate, tri-



J66.1-ø69.2

Octyl sulfide

$[CH_3(CH_2)_6CH_2]_2S$

J72.1-NYR.1-ø59.1-PC5.1-SFA.1

Sulfide, dodecyl phenylmercuri

$C_6H_5HgSC_{12}H_{25}$

J72.1-ø49.1

1-Hexadecanethiol

$CH_3(CH_2)_{15}SH$

J72.1-ø89.1-RGø.1

Ethanethiol, sodium derivative

C_2H_5SNa

J72.3-ø99.1

Orthoformic acid, trithio-

$CH(SH)_3$

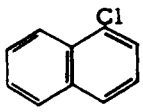
L27.3-NYR.1-ø99.1

Toluene, α,α,α-trifluoro-

$C_6H_5CF_3$

L35.1-NTR.1

Naphthalene, 1-chloro-



L35.1-NYR.1-ø99.1

Toluene, o-chloro-

$ClC_6H_4CH_3$

L37.1-ø89.4-PJ1.1-TCR.1

Phosphonium iodide, (2-chloroethyl)triethyl-

$(C_2H_5)_3\overset{I}{P}CH_2CH_2Cl$

L37.3-NYR.2-ø89.1

Ethane, 1,1,1-trichloro-2,2-diphenyl-

$CCl_3CH(C_6H_5)_2$

L37.3-ø89.3-TJ3.1-U63.3

Phosphorous acid, tris(2-chloroethyl) ester

$P(OCH_2CH_2Cl)_3$

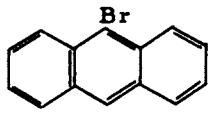
L37.6-ø7P.1

1,3-Butadiene, hexachloro-

$Cl_2C{=}CClC(Cl){=}CCl_2$

L45.1-NKI.1

Anthracene, 9-bromo-



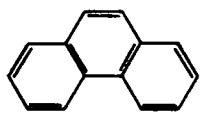
L47.1-ø89.1

Ethane, 1,1,2,2-tetrabromo-

$Br_2CHCHBr_2$

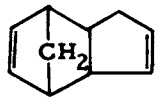
NL9.1

Phenanthrene



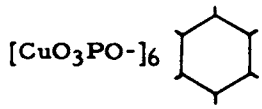
NØN.1

4,7-Methanoindene, 3a,4,7,7a-tetrahydro-



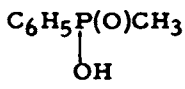
NYK.1-R7N.1-TJ1.6-U63.9

Phytic acid, hexacopper(II) salt



NYR.1-Ø99.1-PJ1.1-RB6.1-U63.2

Phosphinic acid, methylphenyl-



NYR.1-P1J.1-RB6.1-U63.3

Benzenearsonic acid

$C_6H_5AsO_3H_2$

NYR.1-P1J.1-U63.2

Benzene, arso-

$C_6H_5AsO_2$

NYR.1-RB6.1-TJ1.1-U32.1-U63.3

Amidophosphoric acid, N-phenyl-

$C_6H_5NHPO_3H_2$

NYR.1-T2K.1-U32.1-U63.1

Metaboranilide

$C_6H_5NHB{=}O$

NYR.3-Ø89.1-PJ1.1-UZW.1

Phosphazide, N-ethyl-P,P,P-triphenyl-

$(C_6H_5)_3P{=}NN{=}NC_2H_5$

NYR.3-Ø99.3-TJ1.1-U32.3-U63.1

Phosphoramide, N,N',N''-tribenzyl-

$(C_6H_5CH_2NH)_3PO$

NYR.3-Ø99.4

Methane, tri-o-tolyl-

$(CH_3C_6H_4)_3CH$

NYR.3-P1L.1

Arsine, triphenyl-

$(C_6H_5)_3As$

NYR.3-PJ3.1

Phosphine, triphenyl-

$P(C_6H_5)_3$

NYR.3-TJ3.1-U63.3

Phenyl phosphite, tri-

$P(OC_6H_5)_3$

NYR.4-Ø7X.1

Allene, tetraphenyl-

$(C_6H_5)_2C{=}C{=}C(C_6H_5)_2$

NYR.4-PJ1.1-U34.1

Phosphinimide, tetraphenyl-

$(C_6H_5)_3P{=}NC_6H_5$

Ø6Z.1

Butane, 2,2-dimethyl-

$CH_3CH_2C(CH_3)_3$

Ø7I.1-PGØ.1

Sodium, amyl-

$CH_3CH_2CH_2CH_2CH_2Na$

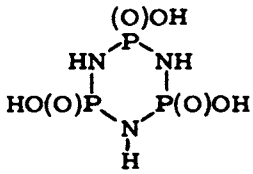
ø89.4-TJ1.2-U63.7

Ethyl pyrophosphate, tetra-

$(C_2H_5O)_2P(O)OP(O)(OC_2H_5)_2$

Q62.1-RB6.1-TJ1.3-U33.3-U63.6

Trimetaphosphimic acid



R12.1-TJ9.1

Aluminum phosphide

AlP

R4N.1-S61.6-T69.1

Calcium chloride, hexahydrate

$CaCl_2 \cdot 6H_2O$

R4N.1-T69.1

Calcium chloride

$CaCl_2$

R6P.1-RDø.1-TNJ.1-U63.4-V61.6

Cobalt(II) potassium sulfate, hexahydrate

$K_2SO_4 \cdot CoSO_4 \cdot 6H_2O$

RB6.1-T69.1

Hydrochloric acid

HCl

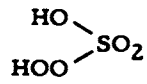
RB6.1-TJ5.1-U01.2-U63.2

Hypophosphorous acid

$HOP(O)H_2$

RB6.1-TNJ.1-U63.3-U67.1

Peroxymonosulfuric acid



RDø.1-RGø.1-T6ø.1-U7V.6-V61.1

Potassium sodium nitrocobaltate(III), monohydrate

$K_2NaCo(NO_2)_6 \cdot H_2O$

RDø.1-TJ1.1-U94.6

Potassium fluophosphate

KPF_6

RGI.1-S01.4-TJ1.1-U94.6

Ammonium fluophosphate

NH_4PF_6

RGø.1-T1J.1-UF3.4-V61.8

Sodium thioarsenate, octahydrate

$Na_3AsS_4 \cdot 8H_2O$

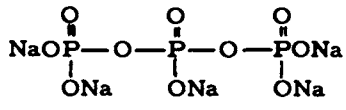
RGø.1-T69.1

Sodium chloride

$NaCl$

RGø.1-TJ1.3-U63.9

Sodium triphosphate



TCN.1-UI4.3

Iodine chloride

ICl_3

TIH.1-UZW.2

Chlorine oxide

Cl_2O

TJ1.1-U63.1-UI4.3

Phosphoryl chloride

$POCl_3$

TN(11).2-UI4.2

Sulfur chloride

S_2Cl_2