NOMENCLATURE

1. Introduction

Chemical nomenclature embraces several subcategories: names for chemical elements and compounds; names for classes of compounds and substances; names for other substances, such as mixtures and composites; names for particles, processes and transformations, properties, effects, units of measurement, techniques, instruments and apparatus, and even for theories and concepts. Only the first three are considered to be the heart of chemical nomenclature; the others are regarded as terminology, although it is often not at all easy to draw a sharp boundary between the two. This article emphasizes the first group, but also provides information about the various compendia of terminology.

The largest part of the subject is the nomenclature of organic compounds, simply because there are so many of them and they are of such diverse nature. The types of compounds and their structures differ considerably among organic, inorganic, and biochemical substances, and each of their respective nomenclatures has developed somewhat differently, although not entirely independently. Macromolecular nomenclature and pharmaceutical nomenclature have practical requirements of their own. It is therefore appropriate to treat each of these several areas separately.

Concern with chemical nomenclature has grown on a broad international scale as the importance of consistent, uniform nomenclature is increasingly recognized. When one compound is known by more than one name or, when one name may refer to more than one compound, serious confusion can result. The effect of such confusion is especially acute in indexes and compilations of names, and it is therefore natural that much of the work in systematizing names of chemical substances has been done in connection with such works. For example, both the Beilstein Institute (1) and the Chemical Abstracts Service (CAS) (2) use International Union of Pure and Applied Chemistry (IUPAC) principles as the basis for their index nomenclature with only slight modification due primarily to indexing considerations. Beginning in 1972, CAS introduced changes in its system designed mainly to reduce the number of variations allowed by the IUPAC rules and recommendations. In the past, the nomenclature of the Royal Society of Chemistry (London) represented a further variant (3-5). Various committees, both national and international, are working toward a consistent, systematic nomenclature. The greatly increased interest of industrial chemists and government agencies continues to be very encouraging. Whereas these groups formerly seemed willing to adopt any name without considering its general acceptability, they now realize that a uniform system of naming is essential to effective handling of information in relation to the many thousands of substances with which they and other groups have to be concerned. Among the areas in which chemical nomenclature plays an increasingly key role are patent law, trade and customs regulations, identification of controlled substances, pharmaceutical and health information, and studies of the environment and pollution.

Fortunately, the basic scheme of most chemical nomenclature in all languages is primarily derived from common sources, the names of the chemical elements and syllables derived from them and Greek and/or Latin numerical prefixes. Thus, there has always been substantial uniformity in overall practice. Nevertheless, differences beyond those inherent in the different languages have caused significant inconvenience (6). For example, some elements are, or have been known, by completely different names in different countries, eg, beryllium versus glucinum, nitrogen versus azote, niobium versus columbium, tungsten versus wolfram, potassium versus kalium, and sodium versus natrium. Other elements have been historically familiar because of their existence in the free state, eg, iron, lead, sulfur, carbon, copper, silver, and gold, have widely different names because they belong to commonly spoken languages, and their use is not at all confined to science and technology. In chemical names, these elements often adopt names derived from Latin roots, eg, ferrate and plumbane, leading to proposals to Latinize element names to agree with their symbols (6), which have met with little success. And the names for some common compounds also differ widely; “water” and “ammonia” are examples.

Partly because of the increasing percentage of the chemical literature that is published in English (7) and the increased worldwide attention paid to international recommendations, these differences have decreased somewhat. For example, recommendations for the adaptation of IUPAC inorganic nomenclature to the German language (8) include such changes as those from “wasserstoff” to “hydrogen” and from the spellings “jod” and “aethyl” to “iod” and “ethyl”, respectively. There are even changes within the English-speaking world; eg, the Royal Society of Chemistry changed the spelling of “sulphur” to “sulfur” in 1992, so that British and American usage would be aligned. Nevertheless, differences in spelling still persist, eg, the American spellings “aluminum” and “cesium” versus the IUPAC spellings “aluminium” and “caesium”.

As early as 1886, an American Chemical Society Committee on Nomenclature and Notation recognized the value of uniform practice among English-speaking chemists by endorsing a system adopted by the British Chemical Society in 1882 (9) with only minor additions and alterations (10). Further progress in British and American agreement was made in 1923, when the nomenclature committees of the two chemical societies adopted 10 rules covering the more commonly disputed points (11). Cooperation between British and American Societies continued through publications of rules for naming phosphorus compounds (12) and carbohydrates (13) by joint committees.

The first international chemical congress was held in Karlsruhe in 1860 (14), but it had little effect on chemical nomenclature. The first effective international consideration of organic nomenclature began in 1889 (15) at an international chemistry conference in Paris, where a report of a Subcommission became the basis for the Geneva Congress in 1892 (16). No further advance was made internationally for many years. In 1913, the Council of the International Association of Chemical Societies met in Brussels and appointed commissions on inorganic and organic nomenclature (17). This initiative ended abruptly with the outbreak of World War I and was not resumed until 1921, when IUPAC appointed commissions on nomenclature of inorganic, organic, and biological chemistry at its Second International Conference in Brussels (18). These commissions subsequently produced many valuable reports and comprehensive recommendations. Their work is ongoing, and involves collaboration with other international and national committees throughout the world. A review of the resulting principles of IUPAC chemical nomenclature has been published (19).

In the United States, the Committee on Nomenclature, Terminology, and Symbols of the American Chemical Society is the clearinghouse for nomenclature recommendations developed by various divisional nomenclature committees of the Society and international nomenclature bodies. Progress is measured not only by improved nomenclature, but also by extension of nomenclature principles to newly developing areas of chemistry and by development of new principles to cope with new types or structures.

Important as names are, they cannot serve all purposes (20). There are other, complementary, means of identifying chemical compounds, eg, structural formulas, notation systems, and registry numbers. None of these is truly nomenclature, however, which is strictly language based. Although structural formulas are sometimes easier to recognize than names, the reverse may also be true. Structural formulas can be space-consuming, troublesome to reproduce, and difficult to arrange in an order useful for retrieval of information. Systems for representing chemical structures by fragmentation coding, topological coding, and linear notation have been developed (21) that have particular advantages for electronic manipulation. Notation systems are more compact than language-based nomenclature, but are less familiar to most chemists and many suffer from the serious disadvantage of being difficult to recognize. Of the various systems, the one originated by Dyson (22) was once adopted by IUPAC, but has been largely abandoned. The system originated by Wiswesser (23) is still widely applied and has catalyzed the development of significant innovations in computerized handling of information about chemical structures. Registry Numbers generated by Chemical Abstracts Service (24) also provide an unambiguous identification for chemical compounds, but they are assigned arbitrarily and therefore have no intrinsic structural information.

2. Element Names and Symbols

Although symbols of the elements are not a part of chemical nomenclature, the two are closely related, and symbols have played an extremely important role in chemistry. Ancient Egyptian inscriptions include hieroglyphics for gold, silver, copper, iron, and lead (25). In the time of alchemy, the known metals were associated with the seven classical planets and the same symbols (which were not letters) were used for both a metal and the corresponding planet. Dalton devised a somewhat similar system based on the circle as a conventional representation of the atom. He and others used symbols to represent composition. Berzelius (26) inroduced the modern, alphabetic symbols, which have become completely international. Interesting accounts of the evolution of chemical symbols have been given (27). Because of the difficulty of establishing priority of discovery for many of the elements of atomic number >100, especially elements 104 and 105, and because of the need to refer to hypothetical elements with higher atomic numbers, IUPAC developed interim symbols and names for such elements (28). For example, element 104 would have the interim symbol Unq, and the name unnilquadium. Guidelines now exist for determing priority of discovery of a new element (29) and for its name to be suggested by the discoverer (30). Accordingly, the names and symbols for the tranfermium elements 104−111 have been established as follows (31-33):

Atomic number	Name	Symbol
101	mendelevium	Md
102	nobelium	No
103	lawrencium	Lr
104	rutherfordium	Rf
105	dubnium	Db
106	seaborgium	Sg
107	bohrium	Bh
108	hassium	Hs
109	meitnerium	Mt
110	darmstadtium	Ds
111	roentgenium	Rg

3. Inorganic Nomenclature

Perhaps no subject in chemical nomenclature has undergone less change during over the twentieth century than inorganic nomenclature. This longevity attests to the fundamental soundness of the original proposals of Guyton de Morveau (34) that established inorganic chemical nomenclature, and those of Werner (35) that extended and broadened its base; it also suggests why inconsistencies and confusions have remained as well, which continue to be disconcerting to chemists. In the past quarter century, however, development of inorganic nomenclature has again accelerated and inconsistencies are being eliminated (36,37).

In the days of alchemy and the phlogiston theory, no system of nomenclature that would be considered logical in the 1990s was possible. Names were not based on composition, but on historical association, eg, Glauber's salt for sodium sulfate decahydrate and Epsom salt for magnesium sulfate; physical characteristics, eg, spirit of wine for ethanol, oil of vitriol for sulfuric acid, butter of antimony for antimony trichloride, liver of sulfur for potassium sulfide, and cream of tartar for potassium hydrogen tartrate; or physiological behavior, eg, caustic soda for sodium hydroxide. Some of these common or trivial names persist, especially in the nonchemical literature. Such names were a necessity at the time; they were introduced because the concept of molecular structure had not been developed, and even elemental composition was incomplete or indeterminate for many substances.

Although Bergman (38) proposed a new chemical nomenclature in 1784 that had some suggestion of system, credit for making the first attempt toward a convenient chemical nomenclature belongs to Guyton de Morveau (34). His pioneer work led to the publication in 1787 of *Methode de Nomenclature Chimique*

(39) written in collaboration with Lavoisier, Berthollet, and Fourcroy, that proved to be a landmark in the development of chemistry. The pioneer work of this committee on nomenclature was widely publicized by the use of its nomenclature in Lavoisier's *Traité Elementaire de Chimie* (1789) (40). The earlier highly unsystematized practices were replaced quickly by this new nomenclature, the general plan of which continues in use today.

Although Boyle clearly stated the concept of an element in 1661, Lavoisier was the first to regard a substance as an element until it was shown to be otherwise and also the first to compile a list of the known elements. The fundamental principle of the new nomenclature was that the name of a compound should specify the elements involved and their relative proportions, if known. The combinations of oxygen with other elements played a dominant role. Thus, the product of the union of a simple nonmetallic substance with oxygen was called an acid and that of the union of a metal with oxygen was called an oxide. The union of an acid and an oxide produced a salt. Acids or oxides were given names in which the generic part was the word "acid" or "oxide" and the specific part was an adjective derived from the name of the other element, eg, *acide sulfurique* and *oxide plombique* (sulfuric acid and lead oxide). The same principle resulted in names for sulfides and phosphides. The resemblance to the binomial nomenclature system for classifying plants and animals originated by Linnaeus is obvious.

In cases where a substance combines with oxygen to produce more than one acid or oxide, a clear distinction was drawn by modifying the ending or by adding a prefix derived from Greek, eg, *acide sulfureux* and *acide sulfurique* for sulfurous and sulfuric acids; *oxide de plomb blanc* and *oxide plombique* for lead monoxide and lead dioxide; and dinitrogen oxide, nitrogen dioxide, and dinitrogen pentoxide.

The names adopted for salts consisted of a generic part derived from the acid and a specific part from the metallic base: l'oxide de plomb + l'acide sulfurique → le sulfate de plomb. The names for salts of acids containing an element in different degrees of oxidation were given different endings: *sulfite de soude* and *sulfate de soude* for sodium sulfite and sulfate, respectively; and *nitrite de baryte* and *nitrate de baryte* for barium nitrite and nitrate, respectively.

Berzelius (41) further applied and amplified the nomenclature introduced by Guyton de Morveau and Lavoisier. It was he who divided the elements into metalloids (nonmetals) and metals according to their electrochemical character, and the compounds of oxygen with positive elements (metals) into suboxides, oxides, and peroxides. His division of the acids according to degree of oxidation has been little altered. He introduced the terms anhydride and amphoteric and designated the chlorides in a manner similar to that used for the oxides.

This system of nomenclature withstood the impact of later experimental discoveries and theoretical developments that have, since the time of Guyton de Morveau and Lavoisier, greatly altered the character of chemical thought, eg, the atomic theory (Dalton, 1802), the hydrogen theory of acids (Davy, 1809), the dualistic theory (Berzelius, 1811), polybasic acids (Liebig, 1834), Periodic Table (Mendeleev and Meyer, 1869), electrolytic dissociation theory (Arrhenius, 1887), and electronic theory and modern knowledge of molecular structure.

The nearly literal translation of the French terms into English, Russian, and other languages resulted in the system whose use has become standard practice in English-speaking as well as other countries. The system has been molded by the fact that elemental composition and valence (or oxidation number) are the principal variables for most inorganic compounds other than the most complex, whereas connectivity and the possibility for isomers have been of little concern. Binary compounds are systematically designated by two words, the first referring to the more electropositive constituent and the second, ending in -ide, referring to the more electronegative constituent, eg, sodium chloride. In cases where the metal exhibits two oxidation states, the lower is indicated by the termination -ous and the higher by -ic, as in cuprous oxide and cupric oxide. Many ternary compounds that contain well-established groups are named as though they were binary compounds, eg, sodium hydroxide, ammonium nitrate, and calcium cyanide (the name cyanate indicates that the compound contains an oxygen atom, in contrast to cyanides, eg, NaOCN, sodium cyanate).

Ternary compounds are also named by citing the more electropositive constituent first. The various oxidation states of the more electropositive element are designated by a system of prefixes and terminations added to a stem characteristic of the element, except in the case of coordination compounds. Examples are given in Table 1.

There are numerous situations in which the foregoing system does not meet all requirements. In the formation of binary compounds, several elements exhibit more than two states of oxidation. One method, recommended by IUPAC (36), for handling these situations, is the use of prefixes derived from Greek numerical terms to indicate stoichiometric composition, eg, titanium dichloride, $TiCl_2$; titanium trichloride, $TiCl_3$; titanium tetrachloride, $TiCl_4$; dinitrogen oxide (nitrous oxide), N_2O; (mono)nitrogen (mon)oxide (nitric oxide), NO; dinitrogen trioxide, N_2O_3; dinitrogen tetraoxide, N_2O_4; and dinitrogen pentaoxide, N_2O_5. Other accepted methods of indicating proportions of constituents are the Stock (oxidation number) system (42) and the Ewens-Bassett (charge number) system (43), eg, titanium(II) chloride and titanium(2+) chloride, respectively.

Some elements form acids with more than four oxidation states, requiring other combinations of prefixes and suffixes: $H_4P_2O_6$, intermediate between H_3PO_3 and H_3PO_4, is known as hypophosphoric acid, and the salts M_2FeO_3, intermediate between M_2FeO_4 and $MFeO_2$, are sometimes called perferrites. Here the oxidation number and charge number systems offer advantages, eg, diphosphoric(IV) acid and disodium ferrate(2−), respectively. Ortho-, meta-, and pyro- prefixes or numerical prefixes may also be used to denote stages of hydroxylation of acids (see). In many instances, special names have been created to deal with unusual situations, eg, the thionic and thionous acids, $H_2S_xO_6$ and $H_2S_xO_4$ ($x \geq 2$), eg, dithionous acid, an alternative to hyposulfurous acid, for $H_2S_2O_4$; nitroxylic acid, H_2NO_2, in place of hydronitrous acid; and diphosphoric(III,V) acid for $(HO)_2P{-}OP(O)(OH)_2$.

The nomenclature system of Guyton de Morveau and co-workers was designed specifically for oxygen compounds. As early as 1826, it became evident that the halogens could play much the same role in many other compounds as oxygen does in the familiar oxygen salts (44). By 1840, Hare was writing of chloro acids and chloro bases, and recognized several classes of salts: oxy-, sulfo- (now called thio-), seleni-, telluri-, chloro-, fluoro-, cyano-, etc (45). Remsen was a proponent of this system of nomenclature (46), but it received its fullest treatment from Franklin (47) in connection with his concept of systems of compounds (48).

The analogies are shown by the following reactions:

$$\begin{aligned}
K_2O + B_2O_3 &\rightarrow K_2O \cdot B_2O_3 \ \text{ or } \ 2\ KBO_2\\
K_2S + B_2S_3 &\rightarrow K_2S \cdot B_2S_3 \ \text{ or } \ 2\ KBS_2\\
KF + BF_3 &\rightarrow KF \cdot BF_3 \ \text{ or } \ KBF_4\\
K_3N + BN &\rightarrow K_3N \cdot BN \ \text{ or } \ K_3BN_2
\end{aligned}$$

The products resulting from such reactions should, therefore, have analogous names. If KBO_2 is a borate, KBS_2 is a thioborate and $KBF_4$is a fluoroborate. Similarly, the replacement of an oxygen atom by a sulfur atom or two fluorine atoms is understandable. However, the relationship of K_3BN_2 is less obvious, until one considers the dehydration and deammoniation schemes:

$$\begin{aligned}
B(OH)_3 &\xrightarrow{-H_2O} OBOH\\
B(NH_2)_3 &\xrightarrow{-NH_3} HNBNH_2
\end{aligned}$$

Formally, both of the resulting compounds are borates. Franklin encountered difficulty in choosing a suitable prefix to indicate that the substance K_3BN_2 was a salt of a boric acid containing nitrogen in the same sense that KBS_2 was a salt of a boric acid containing sulfur. The prefix nitro- had been in use for a long time, with a quite different meaning. Because these compounds are best studied in liquid-ammonia solution, Franklin called them ammono salts and the corresponding oxygen salts aquo salts. Although this practice probably prevented general adoption of his scheme of nomenclature for nitrogen compounds, the names thio-, chloro-, etc, did become widespread, especially for sulfur and halogen compounds. On this basis, there is no inconsistency in calling KPF_6 a phosphate even though the analogous oxygen compound, K_3PO_4, has a formula of different appearance, and one cannot be derived from the other by simple substitution.

Although the foregoing pattern of nomenclature is useful, it does lead to some difficulties. Many quaternary compounds contain oxygen and another electronegative element. In the series M_2CO_3, M_2CO_2S, M_2COS_2, and M_2CS_3, the names are carbonates, (mono)thiocarbonates, dithiocarbonates, and trithiocarbonates, respectively. However, in practice both the prefixes mono- and tri- are often omitted, and it is uncertain whether the omission signifies the mono- or the completely substituted compound; eg, consider thiosulfate, $S_2O_3{}^{2-}$, and chloroplatinate, $PtCl_6{}^{2-}$. The situation is somewhat more complicated when oxygen and fluorine are present in the same compound, because one is bivalent and the other univalent, and the coordination number toward fluorine is different from that toward oxygen: H_3PO_4, H_2PO_3F, HPO_2F_2, and HPF_6. Furthermore, investigators have not always been consistent in choosing the same reference state for the names of the oxygen salts and the halogen salts. Thus, for rhenium(IV), the salts M_2ReO_3 are known as rhenites, whereas the chloro salts, M_2ReCl_6 are known as chlororhenates. A further variant is represented by the name chlorosulfonic acid, a name used by organic chemists for $ClSO_3H$, and chlorosulfuric acid, the name for the same coupound preferred by inorganic chemists. The name chlorosulfonic acid is considered to be derived by the principle of substitution; chlorine replaces hydrogen in the hypothetical compound HSO_3H whereas in chlorosulfuric acid, chlorine replaces OH in $(HO)_2SO_2$ (H_2SO_4). Only a few other inorganic compounds have been named in such ways; the examples chlorochromic acid, $HCrO_3Cl$, and fluorophosphoric acid are analogous to the latter type of name. Names such as ferrocyanide and ferricyanide are archaic remnants of a time when all such species were regarded as double salts, but they are in common use owing to convenience.

The approach of Werner (35) to the problem of naming ternary and higher order compounds is based on an entirely different point of view. By considering all such substances as complex or coordination compounds, he succeeded in naming a wide variety of compounds according to a single general pattern. To designate the oxidation state of the element serving as the center of coordination, Werner chose the characteristic endings suggested by Brauner (49), but these have been totally superseded by the Stock (oxidation number) (42) and/or the Ewens-Bassett (charge number) (43) systems.

The main essentials of the Werner scheme (35) are given here by example using Stock numbers (42) and Ewens-Bassett numbers (43) (see below).

Formula[a]	Name
$[Cr(NH_3)_6]^{3+} (NO_3)_3$	hexaamminechromium(III) nitrate hexaamminechromium(3+) nitrate
$[Pt(H_2O)_2(NH_3)_4]^{4+}(Cl^-)_4$	diaquatetraammineplatinum(IV) chloride diaquatetraamineplatinum(4+) chloride
$[CoCl(NO_2)(en)_2]^+Br^-$	chloronitrobis(ethylenediamine)cobalt(III) bromide chloronitrobis(ethylenediamine)cobalt(1+) bromide
$HAgCl_2$	hydrogendichloroargentate(I) dichloroargentic acid
$Na_2(SSO_3)^{2-}$	sodium thiotrioxosulfate(VI) sodium thiotrioxosulfate(2$^-$)

[a] Ethylenediamine = en.

Stock sought to correct many nomenclatural difficulties in Werner's system by introducing Roman numerals in parentheses to indicate the state(s) of oxidation (42), eg, titanium(II) chloride for $TiCl_2$, iron(II) oxide for FeO, titanium(III) chloride for $TiCl_3$, iron(III) oxide for Fe_2O_3, titanium(IV) chloride for $TiCl_4$, and iron(II,III) oxide for Fe_3O_4. In this system, only the termination -ate is used for anions, followed by Roman numerals in parentheses. Examples are potassium manganate(IV) for K_2MnO_2, potassium tetrachloroplatinate(II) for K_2PtCl_4, and sodium hexacyanoferrate(III) for $Na_3Fe(CN)_6$. The cypher 0 indicates a neutral central atom. Thus a set of prefixes and terminations becomes unnecessary.

The Stock (oxidation number) system is easily extended to include other coordination compounds. Even the interesting substances represented by the formulas $Na_4Ni(CN)_4$ and $K_4Pd(CN)_4$ create no nomenclature problems; they become sodium tetracyanonickelate(0) and potassium tetracyanopalladate(0), respectively.

The oxidation state of an atom as expressed by the oxidation number is a formal concept for partitioning the electric charge between atoms in a molecule or chemical structure. For many chemical structures, this formal procedure may lead to representations of charge distribution that are inconsistent with experiment. Therefore, Ewens and Bassett (43) proposed to express only the total charge on an ion without representing valence and its associated arbitrariness of assigning electronic distribution within a given structure. Examples include titanium(2+) chloride for $TiCl_2$; titanium(3+) chloride for $TiCl_3$; potassium tetrachloroplatinate(2−) for K_2PtCl_4; and sodium tetracyanonickelate(4−) for $Na_4Ni(CN)_4$.

Negatively coordinated groups are given before neutral coordinated groups in the examples of Werner's names above. Ewens and Bassett presented good reasons why that order should be reversed. The IUPAC rules (36) recommend that ligands be cited in alphabetical order regardless of their anionic, cationic, or neutral nature. Other applications of the Stock (oxidation number) (42) and Ewens-Bassett (charge number) (43) systems are specified in the rules.

Coordination nomenclature is also extended to neutral, ie, uncharged compounds. The ligands are cited in alphabetical order, followed by the name of the central atom (generally a metal), without spaces. Examples are tetraethyllead for $Pb(C_2H_5)_4$, (dimethylamido)pentafluorotungsten for $WF_5[N(CH_3)_2]$, and dichlorodiethyltin for $Cl_2Sn(C_2H_5)_2$. Additional methods for indicating metal-to-metal attachments and the distribution of ligands in unsymmetrical compounds have been added, making coordination nomenclature useful for organometallic compounds.

The first report of the Commission for the Reform of the Nomenclature of Inorganic Chemistry was written in 1926 by Delépine (50). Its work was continued by the IUPAC Commission on Nomenclature of Inorganic Chemistry (CNIC) through the appearance of several reports, followed in 1940 by a comprehensive set of rules (51) that were well received. These led to the 1959 rules (52), the first edition of the IUPAC Nomenclature of Inorganic Chemistry, which in turn underwent further evolution producing a second edition, the 1970 report (53). The CNIC continued to produce reports on nomenclatue for inorganic boron compounds in 1972 (54); nomenclature for isotopically modified inorganic compounds in 1981 (55); nomenclature for nitrogen hydrides and their derived anions, cations, and ligands in 1982 (56); nomenclature for polyanions in 1887 (57); and, in collaboration with the IUPAC Commission on Macromolecular Nomenclature, nomenclature for regular and "quasi" single-strand inorganic and coordination polymers in 1985 (58). In 1990, a third edition of the IUPAC Nomenclature of Inorganic Chemistry was published (36); it also included expanded documentation for naming inorganic stereoisomers as well as the names for hydrogen atoms, ions, and groups published by the IUPAC Commission on Physical Organic Chemistry (59). These recommendations retained most of the well-established names for binary and pseudobinary compounds and the oxoacids of the nonmetals and their derivatives. Examples are potassium chloride, KCl; manganese dioxide, MnO_2; hydrogen sulfide, H_2S; phosphorus trichloride, PCl_3; phosphoryl chloride, $POCl_3$; and perchlorate, ClO_4^-. Alternatives are offered based on coordination nomenclature, but they are not meant to supersede the customary names. Examples of these are hydrogen trioxonitrate, HNO_3; dioxonitrate(1−), NO_2^-; and tetraoxomanganic(VI) acid, $HMnO_4$. Such alternatives are useful in naming less common and more complex substances. For some of these another innovation is offered, in which all groups attached to the central atom are indicated by coordination nomenclature, eg, hydroxotrioxorhenium(VII), $(HO)ReO_3$, otherwise known as perrhenic acid. In coordination names for oxoacids, O is always designated oxo, and HO hydroxo. Traditional parent hydride names are retained for certain inorganic hydrides, eg, hydrazine, N_2H_4; silane, SiH_4; diborane(6), B_2H_6; and phosphine, PH_3. Traditional names for some groups or ions are also retained, eg, nitrosyl, NO; uranyl, UO_2; and chromyl, CrO_2. Any other charged and neutral chemical entities, especially those containing a central metal surrounded by groups that may be ions, radicals, or molecules, are named according to the rules for coordination compounds.

Elemental composition, ionic charge, and oxidation state are the dominant considerations in inorganic nomenclature. Connectivity, ie, the number of atoms linked by bonds to other atoms, has not generally been considered to be important, and indeed, in some types of compounds, such as cluster compounds, it cannot be applied unambiguously. However, when it is necessary to indicate connectivity, italicized symbols for the connected atoms are used separated by an "en" dash, as in trioxodinitrate(*N*–*N*), for $O_2N{-}NO^{2-}$. The nomenclature that has been presented applies to isolated molecules (or ions). For substances in the solid state, which may have more than one crystal structure, with individual connectivities, two devices are used. The name of a mineral that exemplifies a particular crystal structure, eg, rutile or perovskite, may be appended. Alternatively, the crystal structure symmetry, eg, rhombic or triclinic, may be cited, or the structure may be stated in a phrase, eg, face-centered cubic.

Guidance in the use of the IUPAC rules (60) as well as explanations of their formulation (61) are available. Further publications of the IUPAC Inorganic Nomenclature Commission include nomenclature for inorganic chain and ring compounds (62), inorganic radicals (63), and names for muonium and hydrogen atoms and their ions (64). A second volume of the IUPAC *Nomenclature of Inorganic Chemistry* has been published (37); it includes the specialized topics, isotopically modified inorganic compounds (55), nitrogen hydrides and their ions and ligands (56), polyanions (57), inorganic chains and rings (62), and single strand inorganic and coordination polymers (58) along with nomenclature for metal complexes of tetrapyrroles and graphite intercalation compounds.

Other contributions to inorganic nomenclature are available (65). A review of IUPAC principles for inorganic nomenclature appears in the book *Principles of Chemical Nomenclature* (19).

Finally, a complete revision of the IUPAC *Nomenclature of Inorganic Chemistry* is in the final stages of preparation. Publication is planned for 2005.

4. Organic Nomenclature

Modern organic nomenclature can be better understood by first tracing its development. Organic substances played a minor role in the *Methode de Nomenclature*

Chimique, published by Guyton de Morveau, and his co-authors in 1787, that became the basis for subsequent inorganic nomenclature (39). Eighteen organic acids were given their present names (succinic, malic, etc), and several classes and other substances were mentioned, such as alcohols, ethers (including esters as well as true ethers), starch, gluten, and camphor. Gaseous hydrocarbons, the only ones included, were lumped together as carbonated hydrogen gas. Thus, a few common names were incorporated into the new method, but no systematic organic names were possible because of lack of knowledge. Little else could be done, for the basis for determining elemental composition, as in empirical formulas, did not yet exist.

The practice of assigning ad hoc names to organic compounds was neither avoidable, nor burdensome, when only a small number of compounds were recognized. Such ad hoc names are termed “trivial” or “traditional”, to indicate that they contain no encoded structural information. They are useful for common compounds, and many of them are retained to this day, but they are not usually helpful in understanding chemical relationships. As trivial names proliferated, the number and variety became unmanageable. The development of systematic nomenclature was driven by this circumstance, and was made possible by advances in understanding and determining the structure of molecules.

Systematic nomenclature is in essence a scheme for encoding structural information in a name. For organic chemistry, it probably began when Gay-Lussac noted in a lecture that the reaction of chlorine with oils produced hydrochloric acid and a substance in which “a part of the chlorine...takes the place of the hydrogen which is removed” (66), an obvious observation of the principle of substitution. Radical names such as benzoyl (C_6H_5CO- in a modern formula) (67) were suggested, thus coining the ending -yl (from the Greek *hyle*, meaning stuff or material), one of the most useful suffixes in chemistry. By a radical or compound radical, Liebig and Wöhler meant a group of atoms that remained unaltered in chemical transformations. The word group is used for almost any portion of a molecule considered as a unit for convenience in naming or otherwise. The names ethyl (68) and methyl (69) soon followed. These names, benzoyl, a group derived from an acid (an acyl radical), and ethyl and methyl (alkyl radicals), may be regarded as the progenitors of the host of group names used today. From these names it was an easy step to form the combinations benzoyl chloride, ethyl iodide, ethyl oxide, etc, many of which still survive. These “binary names” are analogous to the binary inorganic names introduced in inorganic nomenclature in 1787 (39).

It was many years before organic nomenclature shook off the influence of electrochemical theory and its binary names. Gradually, as facts accumulated, it became clear that this theory must give way to a unitary conception of a molecule. At the same time, the phenomenon of substitution, or replacement of one atom or group of atoms by another, was recognized to be of major importance. Some binary names are still used, either as a true expression, as for salts, or for convenience, as in ethyl sulfide or acetyl chloride, but for the most part the principle of substitution is used without regard to whether such replacement can actually be effected experimentally. Usually, the atom replaced is hydrogen and the replacement may be indicated by either a prefix or a suffix. Thus, in naming CH_3-Cl chloromethane rather than methyl chloride, the replacement of one atom of hydrogen in methane, CH_4, by chlorine is indicated. The name methanol for $CH_3{-}OH$ indicates that one hydrogen atom of methane has been replaced by a hydroxyl group, the characteristic group of alcohols, and is denoted by the suffix -ol. A third group of names is formed by combining a class name with a specific word, as in ethyl alcohol or benzophenone oxime. Whatever the method or combination of methods used, there must be a name for a parent compound to form a basis for the derivative. This may be a trivial, traditional, or common name, such as "camphor" or "aspirin", as distinguished from a semisystematic or systematic name, or it may be partly systematic name, such as "butane", pentane, or acetic acid, or a more systematic name, such as disilane or azepine. Such methods show how, because of its inherent problems, organic chemical nomenclature is different from that of botany and zoology or mineralogy, and even from inorganic chemistry.

By 1866, based on earlier proposals, it was possible for Hofmann (70) to arrange hydrocarbons in series by their empirical formulas, ie, methane, CH_4, and methene, CH_2; ethane, C_2H_6, ethene, C_2H_4, and ethine, C_2H_2; propane, C_3H_8, propene, C_3H_6, and propine, C_3H_4; and quartane, C_4H_{10}, quartene, C_4H_8, and quartine, C_4H_6. These become known as Hofmann-Gerhardt names.

Hofmann's scheme has been modified by replacing quartane with butane and continuing the homologous series using Greek numerical terms with the ending "ane", eg, pentane, hexane, etc, which are still used. For the C_nH_{2n} series, ie, the olefins, the names methylene, ethylene, propylene, etc, came into use instead of Hofmann-Gerhardt terms, but the names propene, butene, pentene, etc., were revived in the Geneva system (16) and are the preferred terms. For C_2H_2, ethine has never replaced the older term acetylene, but propine, butine, etc, reappeared in the Geneva system (16). The ending -yne replaced -ine, as in propyne, etc, to avoid confusion with the ending -ine of organic bases such as aniline. The Hofmann-Gerhardt names did not distinguish between isomers. This defect proved decidedly negative for their future use, for it was soon realized that a central requirement of nomenclature for organic compounds was to express connectivity and isomerism. The requirements of organic nomenclature thus differ fundamentally from those of inorganic nomenclature for simple compounds. Different methods of distinguishing isomers arose: $CH_3CH_2CH_2CH_3$ became normal butane (abbreviated to *n*-butane), and $CH_3CH(CH_3)_2$ isobutane, or trimethylmethane. For olefins, $CH_2{=}CHCH_2CH_3$ became α-butylene or ethylethylene; $CH_3CH{=}CHCH_3$ was β-butylene, or symmetrical (abbreviated to *sym*) dimethylethylene; and $CH_2{=}C(CH_3)_2$ was isobutylene, or unsymmetrical (abbreviated to *unsym*) dimethylethylene. It thus becomes evident that as the number of carbon atoms, and therefore the number of isomers increases, the coining of such names meets with insuperable difficulties. The situation with regard to hydrocarbons had its parallel in the nomenclature of alcohols and other types of compounds.

Until nearly the end of the nineteenth century, only limited attempts were made to meet the needs of chemical nomenclature systematically; for the most part, authors followed their own ideas. The state of affairs finally became so confused that an international congress, held in connection with the Paris Exposition of 1889, appointed an International Commission for the Reform of Chemical Nomenclature (15) at which resolutions, were accepted that became known as the basis of the Geneva system (16), were adopted. Mention of only a few of the 34 participants from nine countries is sufficient to indicate the Commission's authority: H. E. Armstrong and J. H. Gladstone from Britain, C. Friedel and M. L. Bouveault from France, and A. von Baeyer and E. Fischer from Germany.

The Geneva Conference was strongly influenced by the need for names that would be suitable for systematic indexing of organic compounds. The groundwork was laid by a French subcommission of the International Commission for the Reform of Chemical Nomenclature noted above (15). One of the chief principles of the Geneva system was the selection of the longest straight chain of carbon atoms in the molecule as a parent structure. Thus the names butane, pentane, etc, would refer to the normal (unbranched) isomers only. This parent hydrocarbon could then be modified by attaching to its name one or more prefixes or suffixes to specify chemically characteristic features (commonly termed functional groups, a term replaced in modern times by characteristic groups). A representative selection is given in Table 2.

For simple compounds, this was all that was necessary, as in the name ethanol (ethane plus the suffix -ol) for $CH_3CH_2{-}OH$, because only one isomer was possible. When two or more different positions of attachment of a prefixed or suffixed group exist, a position designator, called a locant, is necessary. These are usually arabic numerals, set off by hyphens, starting with "1" at an end of the chain. Accordingly, $CH_3CH{=}CHCH_3$ became 2-butene, and $CH_3CH_2CH(OH)CH_2CH_3$ became 3-pentanol. The position of the locants was permissive, providing that there was no ambiguity, and pentan-3-ol or pentanol-3 was considered equally acceptable. In the 1993 *Guide to IUPAC Nomenclature of Organic Compounds* (71), however, the official IUPAC recommendation is to place the locant immediately before the feature that it describes, as in but-2-ene and pentan-3-ol for the foregoing examples. Branching of a carbon chain is handled in an analogous manner, by citing and locating the branch, as in $CH_2{=}CHCH_2CH\ (CH_3)_2$, 4-methylpent-1-ene. In special cases, a letter locant, the italicized symbol for an element, is used to indicate attachment to an atom other than carbon, as in *N*,*N*-dimethylacetamide, $CH_3CON(CH_3)_2$. This was a great advance, as complex hydrocarbons of various kinds could be clearly named if their structures were known. The Geneva system, modified and expanded by subsequent Commissions, is used systematically in the fourth and fifth editions of *Beilstein's Handbuch der Organischen Chemie* (1), and as the basis of CAS and IUPAC nomenclature. In 1992, a commemorative symposium on the centennial anniversary of the Geneva Conference was held in Geneva (72).

The original Geneva rules found only partial acceptance for they were far from complete, relating chiefly to acyclic compounds, and did not meet problems raised by subsequent discoveries. The next important step was the *Definitive Report of the Commission on the Reform of the Nomenclature of Organic Chemistry*, adopted by the Commission and by the Council of the International Union of Chemistry in 1930 at a meeting in Liège (73). This report used the Geneva rules as a basis for modification, but many of the 68 Liège rules dealt with topics not touched in the original Geneva report.

A major provision of the Liège *Definitive Report* was that only one kind of characteristic group (function), the principal characteristic group (the principal function) should be expressed by the ending of the name, ie, by a suffix. The others, if there are any, are designated by prefixes (Rule 51, Ref. (73)). Thus $CH_3CH(OH)COCH_3$ was not to be called butan-3-ol-2-one, but 3-hydroxy-2-butanone. Another important modification of the Geneva system was that the fundamental chain used as the parent structure in an aliphatic compound would not necessarily be the longest chain in the molecule, but it must be the longest chain of those containing the maximum number of occurrences of the principal characteristic group (Rule 18, Ref. (73)). This shifted the emphasis for generating names from side chains, such as methyl and ethyl, to functional groups, such as $-COOH$ and $-OH$. Rules 14–16 (73) dealt with parent heterocyclic compounds, and Rule 16 (73) gave recognition to the skeletal replacement ("a" or oxa–aza) method of nomenclature. This system is based on hydrocarbon names and is extensively used in naming of heterocycles and long-chain acyclic compounds containing heteroatoms. An example of the latter is the name 3,6,9,12-tetraoxatetradecan-1-ol for $CH_3CH_2O(CH_2CH_2O)_3CH_2CH_2-OH$, as an alternative to the conventional type of substitutive name, 2-{2-[2-(2-ethoxyethoxy)ethoxy]ethoxy}ethanol. Sections B and C of later IUPAC rules (71,74,75) extended this type of nomenclature.

The concept of the principal characteristic group raises the question of how priority is determined when two or more different characteristic groups are present. No arbitrary rule can be entirely satisfactory, but an order has been codified in IUPAC recommendations (71,74,75), and an essentially similar order is used by Chemical Abstracts Service (CAS) (2). This order was developed by Patterson and Curran on the basis of literature usage (76). The use of prefixes and suffixes for distinguishing the various radicals, groups, and functions has caused some problems, because some groups, eg, HS–, have been known by more than one name, and some names, eg, anisyl, have had more than one meaning. The Liège *Definitive Report* (73) includes only a limited number of prefixes and suffixes. Chemical Abstracts Service publishes its own lists in the Appendices to its *Index Guide*, the latest appearing in 2002 (2). A formally approved list of prefixes and corresponding suffixes, together with rules for their formation, has appeared in IUPAC publications (74,75); the most recent version can be found in the *Guide to the Use of IUPAC Nomenclature of Organic Compounds* (71). An important departure from earlier recommendations is that the systematic names of acyl groups derived from carboxylic acids must end in "-oyl"; common traditional or trivial names, such as acetyl and oxalyl, are excepted. The purpose of this rule is to distinguish unambiguously between hydrocarbyl groups and acyl groups. Thus, anisyl can only mean methoxyphenyl, whereas anisoyl refers only to methoxybenzoyl.

The ending "-yl" (or -"oyl") is standard for univalent groups (with certain traditional exceptions, such as succinyl). It may be combined with a syllable for unsaturation, as in propenyl, $CH_3CH{=}CH-$, or ethynyl, $CH{\equiv}C-$. The ending "-ylene" is one device for denoting a bivalent group in which the two free valences are on different atoms, but, with the exception of methylene, $-CH_2-$, ethylene, $-CH_2CH_2-$, and phenylene, $-C_6H_4-$, the ending "-diyl", with locants as appropriate, is preferred, as in propane-1,3-diyl, $-CH_2CH_2\ CH_2-$. When the two free valences of a bivalent group form a double bond, the ending is "-ylidene", as in ethylidene, $CH_3CH{=}$. For a trivalent group forming a triple bond, the ending is "-ylidyne", as in ethylidyne, $CH_3C{\equiv}$.

Numerical terms are used to indicate the number of atoms or groups of the same kind. The prefixes “di-”, “tri-”, “tetra-”, etc, are used when the expressions are simple, eg, “dichloro”, and “dimethyl”; the prefixes “bis-”, “tris-”, “tetrakis-”, etc, are used when the expressions are complex or when the use of “di-”, “tri-”, etc, would be ambiguous, eg, “bis(dimethylamino)” and “bis(silyl)”. Numerical terms through 9999 were published in 1986 (77). The prefix “bi-” is used to denote the joining of two cyclic groups of the same kind together, as in biphenyl, $C_6H_5{-}C_6H_5$, or the doubling of a compound with loss of two hydrogen atoms, as in 1,1’-binaphthalene, $1,1'\text{-}C_{10}H_7{-}C_{10}H_7$; it is no longer used to join two acyclic parents, eg, $CH_3CO{-}COCH_3$ is named butane-2,3-dione and not biacetyl.

A historical account of the development of organic nomenclature from the time preceding the Geneva Conference through the publication of the 1965 IUPAC rules (74) and the preliminary rules for Section D (78) is available (79). The IUPAC Commission on Nomenclature of Organic Chemistry has had continuing responsibility for revising and expanding the rules that appeared in the *Definitive Report* (73), until the formation of the new IUPAC Division of Chemical Nomenclature and Structure representation in 2002. Revisions and newly developed sections first published in the journal *Pure and Applied Chemistry* have been collected in book form (71,74,75). These revisions are often based on other significant contributions, such as for organosilicon compounds (80), organophosphorus compounds (12), and stereochemical configuration (81,82). The Hantzsch-Widman system for naming heterocyclic rings has been revised (83); nomenclature of ions and radicals (84), nomenclature for fused ring and bridged fused ring systems (85), and basic terminology of stereochemistry (86) have been dealt with comprehensively. More recently, principles of phane nomenclature (87), and nomenclature for fullerenes (88) have been published. A revision and expansion of Section F of the 1979 edition of the IUPAC nomenclature rules (75) has been published (89). The IUPAC Division of Chemical Nomenclature and Structure Representation (Division VIII), established in 2002 to consolidate the nomenclature activities for IUPAC, has established projects for nomenclature of rotaxanes, catenanes, dendrimers, and an extensive project on recommendations for representing structures. In addition, a new, comprehensive edition of IUPACs *Nomenclature of Organic Chemistry*, one that will provide recommendations for the generation of preferred IUPAC names, should be published in 2006.

For practical reasons IUPAC has always retained a number of trivial, semitrivial (traditional), or common names. With each succeeding edition of the IUPAC recommendations the list of approved retained names has been reduced; the latest list appears in the *Guide to IUPAC Nomenclature of Organic compounds* (71). A very brief selection is shown in Table 3.

Other contributions to organic nomenclature in English are available (2,19,90,91) and many more in other languages (see General References). The first catalog of known ring systems, *The Ring Index*, appeared in 1940 (92); a second edition was published in 1960 (93), which was replaced by the *Parent Compound Handbook* in 1977 (94). Five editions of the *Ring Systems Handbook* followed in 1984, 1988, 1993, 1988, and 2003 (95). Included are the names and numbering schemes for systematically named rings and ring systems, “ocene” compounds, polyboron hydrides, and fullerene cage parents. Diagrams for cyclic and acyclic stereoparent structures are also available (89,96).

IUPAC has also published recommendations for naming organic reactions (97).

Development of computerized approaches to the nomenclature of organic compounds has made great advances in recent years. The first comprehensive computer program to generate names from chemical structures, called AUTONOM, was developed at the Beilstein Institute to take over the generation of names of organic compounds for Beilstein products (98); it is available commercially by MDL Information Systems as an add-on to ISIS/Draw or ISIS/Base packages. Structures are drawn on a computer monitor, and in a few seconds a name compatible with IUPAC recommendations is displayed. For the increasingly small number of organic structures that the program cannot handle, failure is explicitly indicated. It handles (*R*/*S*) stereochemical configurations (81) and topological (*E*/*Z*) configuration at double bonds (82). Early work on the reverse operation, the generation of a structure from a systematic name was carried out at the University of Hull (99). Chemical Abstracts Service has developed a comprehensive program for internal use in handling many phases of index nomenclature generation (100); it has not been made available commercially. Other commercial computer programs for dealing with chemical nomenclature have been developed dealing with both names from chemical structures and chemical structures from names; information can be obtained from the appropriate Web Sites. Nomenclator (name from structure) and NamExpert (structure from name) are from ChemInovation Software and IUPAC NameIt (name from structure) and IUPAC DrawIt (structure from name), part of the Bio-Rad Laboratories KnowItAll Informatics System, claim to produce IUPAC names, but, since the present IUPAC rules do not identify unique or preferred names in all cases, these names clearly are formed according to internal interpretations of the IUPAC rules. CambridgeSoft Corporation markets software for both name to structure (101) and structure to name, which includes sophisticated stereochemistry perception routines and can also deal with isotopically labeled compounds. Advanced Chemistry Development (ACD Labs) software produces IUPAC names for organic compounds together with the appropriate IUPAC nomenclature recommendations; CAS names can also be produced. The ACD Labs programs also derive structures from names, and can handle inorganic compounds and polymers. The IUPAC has developed a computer algorithm for converting a two-dimensional chemical structure drawing into a unique machine-readable identifier (102), which will facilitate linking of diverse data compilations from different sources. It is expected that commercial chemical software developers will incorporate the algorithm into their products.

5. Biochemical Nomenclature

The nomenclature of biochemical compounds is in large measure a part of organic nomenclature; however, the importance of metal complexes involve principles of coordination nomenclature. Biochemical nomenclature does have its own special problems, arising partly from the fact that many biochemical compounds must be given names before their chemical structures have been fully determined, and partly from the interest in grouping them according to biological function as much as to chemical class. Guidelines for names to be used before the structure has been determined as well as guidelines for assigning “semisystematic” names have been formulated (89).

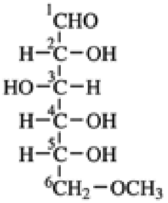
The IUPAC Commission on Nomenclature of Biological Chemistry was established in 1921 (18), along with organic and inorganic commissions. It worked actively and closely with the organic commission. Early subjects of concern were carbohydrates, proteins, enzymes, and fats (103). More recently, this Commission shared its work with a corresponding Commission of the International Union of Biochemistry leading to the formination of a joint IUPAC–IUB Commission on Biochemical Nomenclature (CBN) in 1967 (104). In 1977, CBN was dissolved and the Nomenclature Committee of IUB and the Joint Commission on Biochemical Nomenclature were formed (JCBN) (105); the IUB is now the International Union of Biochemistry and Molecular Biology (IUBMB). The Joint Commission on Biochemical Nomenclature has published many recommendations dealing with the nomenclature of natural products and related compounds including, amino acids and peptides (106), steroids (107), carotenoids (108), prenols (109), retinoids (110),carbohydrates (111), cyclitols (112), lipids (113), tetrapyrroles (114), corrinoids (115), Vitamin D (116), Vitamin B_6 (117), tocopherols (118), quinones with isoprenoid side chains (119), biochemical phosphorus compounds (120), glycolipids (121), glycoproteins, glycopeptides and peptidoglycans (122), folic acid (123), and lignans (124). Most of these recommendations or precursor recommendations are collected in book form (125).

The Joint Commission on Biochemical Nomenclature as well as the Nomenclature Committee of the International Union of Biochemistry have issued a number of recommendations dealing with subjects of a more biochemical nature, such as peptide hormones (126), conformation of polypeptide chains (127), abbreviations for nucleic acids and polynucleotides (128), electron-transport proteins (129), biochemical thermodynamics (130), junctions and branchpoints in nucleic acids (131), and incompletely specified bases in nucleic acid sequences (132).

The Nomenclature Committee of the International Union of Biochemistry and Microbiology has the responsibility for developing the recommendations for naming enzymes. The basic recommendations are contained in *Enzyme Nomenclature* and its five supplements (133). Corrections and additions to the enzyme list now appear on a World Wide Web version (http://www.chem.qmul.ac.uk/iubmb/enzyme/). The Committee also publishes other recommendations related to enzymes, such as enzyme kinetics (134), multienzymes (135), and multiple forms of enzymes (136).

The presence of many chiral centers in compounds of biochemical significance or natural product interest has led to the use of stereoparents (89), parent structures having trivial names that imply (without explicitly expressing) a particular steric configuration. Common examples are the names of the simple sugars, exemplified by glucose. This simplifying nomenclature device is indispensable in carbohydrate and steroid chemistry, among others. The following structure represents 6-*O*-methyl-d-glucose, a specific configuration of 2,3,4,5-

tetrahydroxy-6-methoxyhexanal.



Although it is not strictly within the subject of biochemical nomenclature, it is appropriate to mention the existence of standardized generic names for pharmaceutical drugs. Such names are essentially coined, or trivial, names, but they often include syllables from the systematic organic names, and endings that reflect a structural class, eg, -cillin (from penicillin), or an important area of medical application, eg, -vir (antiviral). Glossaries of these generic names are published periodically (137), and a glossary of United States Approved Names (USAN) is published annually (138).

6. Macromolecular Nomenclature (Polymers)

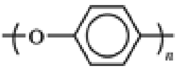
The nomenclature of macromolecules (polymers) can be complicated because there is little or no regularity in the molecules; for such molecules the structural details may also be uncertain. In cases where the macromolecule is a polymeric chain with some uncertainties about regularity in its structure, a simple expedient is to name the polymer based on the monomer(s) that gave rise to it. Thus, there are source-based names such as poly(vinyl chloride).

The first attempt to formulate a systematic nomenclature for polymers was based on the smallest repeating structural unit; it was published in 1952 by a Subcommission on Nomenclature of the IUPAC Commission on Macromolecules (139). The report covered not only the naming of polymers, but also symbology and definitions of terms. However, these nomenclature recommendations did not receive widespread acceptance. Further progress was slow, with a preliminary report on steric regularity in high polymers published in 1962 (140) and updated in 1966 (141).

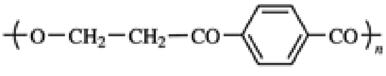
In 1967, the Polymer Nomenclature Committee of the American Chemical Society published proposals for naming linear polymers on the basis of their chemical structure (142), which were then introduced into *Chemical Abstracts* (CA) *Indexes* and published in their final form in 1968 (143).

A Macromolecular Division of IUPAC was created in 1967, and it created a permanent Commission on Macromolecular Nomenclature, paralleling the other IUPAC nomenclature commissions. This Commission over the years has issued recommendations on basic terms of polymer science (144), stereochemical definitions and notations (145), structure-based nomenclature for regular single-strand organic polymers (146), source-based nomenclature for polymers (147) and copolymers (148), nomenclature for double-strand organic polymers (149), irregular single-strand organic polymers (150), abbreviations for polymers, and, in cooperation with the Commission on Nomenclature of Inorganic Chemistry, quasi-single-strand inorganic and coordination polymers (58). These or their precursors are collected in a compendium referred to as the IUPAC Purple Book (151).

Macromolecular nomenclature has two systems, source-based names, eg, polyacrylonitrile, poly(methyl methacrylate), poly(acrylamide-*co*-vinylpyrrolidinone), polybutadiene-*block*-polystyrene, and poly(propyl methacrylate)-*graft*-poly(1-vinylnaphthalene); and structure-based names, eg, poly(oxy-1,4-phenylene) (1), poly(oxyethyleneoxyterephthaloyl) (2), and poly[imino(1-oxo-1,6-hexanediyl)] (3).



(1)



(2)

$\left[\mathrm{NH{-}CO{-}(CH_2)_5}\right]_n$

(3)

The more familiar source-based names for these polymers are poly(phenylene oxide) (1), poly(ethylene terephthalate) (2), and polycaprolactam (3).

The Commission also publishes recommendations in areas related to nomenclature, such as abbreviations for polymeric substances (152), graphic representations of macromolecules (153), and classification and definitions of polymerization reactions (154). Other publications include definitions of terms relating to degradation and aging (155), nonultimate mechanical properties (156), low molar mass and polymer liquid crystals (157), polymer liquid crystals (158), and stereochemically asymmetric polymerization (159).

The Commission is currently working on recommendations for rotaxanes, catenanes, dendrimers, and cyclic structures containing macromolecular units.

7. Nomenclature in Other Areas of Chemistry

A number of glossaries of terms and symbols used in the several branches of chemistry have been published. They include physical chemistry (160), physical organic chemistry (161), and chemical terminology (other than nomenclature) (162). The IUPAC has also issued recommendations in the fields of analytical chemistry (163), clinical chemistry (164), photochemistry (165), colloid and surface chemistry (166), ion exchange (167), spectroscopy (168), atmospheric chemistry (169), toxicology (170), clinical chemistry (171), pesticides (172), chemical kinetics (173), bioinorganic chemistry (174), computational drug design (175), medicinal chemistry (176), combinatorial chemistry (177), and theorectical organic chemistry (178).

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Consultant

Table 1. **Chlorine Oxygen Acids and Salts**

Acids		Salts	
Formula	Name	Formula	Name
$HClO$	hypochlorous acid	$NaClO$	sodium hypochlorite
$HClO_2$	chlorous acid	$NaClO_2$	sodium chlorite
$HClO_3$	chloric acid	$NaClO_3$	sodium chlorate
$HClO_4$	perchloric acid	$NaClO_4$	sodium perchlorate

Table 2. **Suffixes[a] and Prefixes for Some Functional (Characteristic) Groups**

Formula[b]	Class name	Suffix	Prefix	Radicofunctional form
$-CO-OH$	carboxylic acid	-carboxylic acid	carboxy	
$-(C)O-OH$		-oic acid		
$-SO_2-OH$	sulfonic acid	-sulfonic acid	sulfo	
$-SO-OH$	sulfinic acid	-sulfinic acid	sulfino	
$-CO-OR$[c]	esters		alkoxycarbonyl alkyl. . .carb-carboxylate[c]	
$-(C)O-OR$[c]				alkyl. . .-oate[c]
$-CO-X$[d]	acid halide	-carbonyl halide[d]	halocarbonyl[d]	
$-(C)O-X$[d]		-oyl halide[d]		
$-CO-NH_2$	amide	-carboxamide	carbamoyl aminocarbonyl	
$-(C)O-NH_2$		-amide		
$-C\equiv N$	nitrile	-carbonitrile	cyano	alkyl cyanide[c]
$-(C)\equiv N$		-nitrile		
$-CH=O$	aldehyde	-carbaldehyde	formyl	
$-(C)H=O$		-oxo		
$>C=O$	ketone[e]	-one	oxo	dialkyl ketone[c]
$>(C)=O$				
$-OH$	alcohol	-ol	hydroxy	alkyl alcohol[c]
$-SH$	thiol mercaptan[f]	-thiol	sulfanyl mercapto[f]	alkyl hydrosulfide[c] alkyl mercaptan[f]
$-OOH$	hydroperoxide		hydroperoxy	alkyl hydroperoxide[c]
$-NH_2$	amine	-amine	amino azanyl	
$=NH$	imine	-imine	imino	
$-OR$	ether		alkoxy[c] alkyloxy	(di)alkyl ether[c]
$-OO-$	peroxide		peroxy	(di)alkyl peroxide[c]
$-Cl$	chloride		chloro	alkyl chloride[c]
$-NO_2$			nitro	
$>SO_2$	sulfone		sulfonyl	(di)alkyl sulfone[c]
$>SO$	sulfoxide		sulfinyl	(di)alkyl sulfoxide[c]

[a] In the most commonly suggested order of precedence (see text).

[b] Carbon atoms enclosed in parentheses are included in the chain and do not imply additional carbons atoms to a chain.

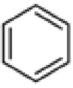
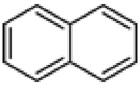
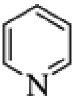
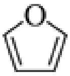
[c] R = alkyl, cycloalkyl, aryl.

[d] X = F, Cl, Br, I, NC, NCO, N_3; halo or halide = fluoro, fluoride; chloro, chloride; bromo, bromide; iodo, iodide; isocyano, isocyanide; isocyanato, isocyanide; azido, azide.

[e] Both bonds of the carbonyl group must be attached to carbon atoms.

[f] Mercaptan and related terms are no longer recommended.

Table 3. **Some Retained Traditional Names Used as Parent Structures**

Formula	Structure	Traditional name	Systematic equivalents
C_6H_6		benzene	
$C_{10}H_8$		naphthalene	
C_5H_5N		pyridine	
C_4H_4O		furan	
C_4H_4S		thiophene	
$C_6H_5{-}OH$		phenol	benzenol
$C_6H_5{-}NH_2$		aniline	benzenamine
$C_6H_5{-}COOH$		benzoic acid	benzenecarboxylic acid
$CH_3{-}COOH$		acetic acid	ethanoic acid
$CH_3{-}CO{-}CH_3$		acetone	propan-2-one
NH_3		ammonia	azane
$H_2N{-}NH_2$		hydrazine	diazane
$HO{-}OH$		hydrogen peroxide	dioxidane
$H_2N{-}CO{-}NH_2$		urea carbamide	carbonic diamide