INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

1957 REPORT OF THE COMMISSION ON THE NOMENCLATURE OF INORGANIC CHEMISTRY

Nomenclature of Inorganic Chemistry

Definitive Rules for Nomenclature of Inorganic Chemistry

AMERICAN VERSION WITH COMMENTS

During the period while these rules were being formulated the Commission was made up of: H. Bassett (*Chairman*, 1947–53), Alexander Silverman (*Chairman*, 1953–7), K. A. Jensen (*Vice Chairman*), G. H. Cheesman (*Secretary*), J. Bénard, N. Bjerrum, E. H. Büchner, W. Feitknecht, L. Malatesta, A. Ölander, and H. Remy

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PREFACE

In addition to members of the Commission on Inorganic Chemical Nomenclature listed above, the present revision is the evolved work of various individuals who have served as regular members of the Commission since the "1940 Rules" appeared. Their names[1] are listed in the volumes of Comptes Rendus, IUPAC, which have appeared since 1940.

Acknowledgment also is made of the coöperation of delegate and advisory members of the Commission, of members of nomenclature committees in a number of nations; also of E. J. Crane, Editor of *Chemical Abstracts*.

The final editing of the 1957 Report is the work of a subcommittee, K. A. Jensen, *Chairman*, J. Bénard, A. Ölander, and H. Remy.

November 1st, 1958

Alexander Silverman, *Chairman*

INTRODUCTION

The Commission on the Nomenclature of Inorganic Chemistry of the International Union of Pure and Applied Chemistry (IUPAC) was formed in 1921, and many meetings took place which culminated in the drafting of a comprehensive set of Rules in 1938. On account of the war they were published in 1940 without outside discussion. At the meeting of the International Union of Chemistry in 1947 it was decided to undertake a thorough revision of what have come to be known as the "1940 Rules," and after much discussion they were completely rewritten and issued in English and French, the official languages of the Union, after the meeting in Stockholm in 1953 as the "Tentative Rules for Inorganic Chemical Nomenclature." These were studied by various national organizations and the comments and criticisms of many bodies and of private individuals were received and considered in Zürich, Switzerland, in 1955, in Reading, England, in 1956, and in Paris, France, in 1957.

The Rules set out here express the opinion of the Commission as to the best general system of nomenclature, although certain names and rules which are given here as a basis for uniformity will probably prove unworkable or unacceptable in some languages. In these cases adaptation or even alteration will be necessary, but it is hoped that it will be possible to keep these changes small and to preserve

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(1) V. Caglioti, G. Chaudron, R. V. G. Ewens, F. Giordani, W. P. Jorrissen, H. I. Schlesinger, W. D. Treadwell, E. Votocek.

the spirit of the IUPAC Rules. The English and French versions, which differ slightly, are to be regarded as international models from which translations will be made into other languages. The latter is likely to prove the better model for the Romance languages, and the former for Germanic languages, but it must be borne in mind that English and French have been used in the two original versions of the report of the Commission as the official languages of the Union and that several nations speak them with quite considerable variations of usage among themselves. There may therefore arise a similar need for adaptation or alteration even among English-speaking and French-speaking peoples, but we hope that in these cases, as in the others, careful consideration will be given to minimizing variation and to preserving the spirit of our international model.

The Commission's aim always has been to produce rules which lead to clear and acceptable names for as many inorganic compounds as possible. It soon became obvious, however, that different users may require the name of a compound to fulfill different purposes, and it has been necessary to effect compromises in order to formulate rules of the most general usefulness. The principal function of a name is to provide the chemist with a word or set of words which is unique to the particular compound and which conveys at least its empirical formula and also, if possible, its principal structural features. The name should be pronounceable and capable of being written or printed with an absolute minimum of additional symbols or modes of writing (*e.g.*, subscripts or differing type faces).

Many inorganic compounds exist only in the solid state and are destroyed on fusion, solution, or vaporization; some chemists have expressed strongly the view that names for such compounds should include information about the structure of the solid in each case as well as its composition. Incorporating all this information tends to make the names extremely cumbersome, and since many of the structures remain uncertain or controversial, such names often must be changed. For general purposes, therefore, it is essential to have as short names as possible, and the Commission has endeavored to produce a system based on the composition and most important properties of substances, avoiding as far as possible theoretical considerations which are liable to change.

Introductory Statement Concerning the Comments

National variations as to certain details of expression have been justified. A few such changes have been made in this American version. No alterations of basic significance have been made. The expression "American version" has been used chiefly because of the comments, made in good will and with the hope that they will prove to be helpful.

The recent appearance of the IUPAC 1957 "Definitive Rules for Nomenclature of Inorganic Chemistry" (published for IUPAC by Butterworths Scientific Publications in London (1959)) marks an important forward step in the development of a comprehensive and systematic inorganic nomenclature. Inorganic chemists owe a debt of gratitude to the members of the Commission on the Nomenclature of Inorganic Chemistry for their long efforts and the successful issue of their labor.

A report such as this, comprising the contributions of many chemists representing many points of view, must of necessity be more a reflection of approved and established practices and the best compromises among these differing points of view and various national usages rather than the ideal of an integrated systematic set of nomenclature rules. But because the rules are a codification of recommended present procedures, they should find acceptance by most chemists and should provide a good basis for future development.

It should be realized that the report must stop short of many questions of detail which are probably best handled within the framework of each language and established national usage. This viewpoint has led to some adaptations to American practice, as exemplified in publications of the American Chemical Society. These adaptations include changes in styling (as spelling, separation of some one-word names into two words, and more liberal use of parentheses in some names) and occasional changes in wording to improve clarity.

Greater harmonization of inorganic and organic nomenclature practices is much to be desired. A joint committee of the IUPAC organic and inorganic nomenclature commissions has been appointed for such a purpose. Some of the overlapping areas (as organometallic compounds) are among those which will require extension of these Rules at some future date. These are areas which have become active within the past few years or in which significant advances in our understanding have recently taken place and are presently continuing. Nomenclature committees in the United States are currently studying some of the areas where more work is indicated, in the hope that the results of their studies may be considered at the international level with a view to still further improvement.

The Definitive Rules were carefully considered by the Subcommittee on Nomenclature of Inorganic Chemistry of the Division of Chemistry and Chemical Technology of the National Research Council and the Committee on Nomenclature of the Division of Inorganic Chemistry of the American Chemical Society. This work was done by correspondence and by conferences at the 137th and 138th meetings of the American Chemical Society in April and September, 1959, respectively. Tentative adoption of the Rules has been recommended by the above committees to the National Research Council, Committee on Nomenclature (Charles D. Hurd, *Chairman*) of the Division of Chemistry and Chemical Technology, and to the American Chemical Society, Committee on Nomenclature, Spelling, and Pronunciation (Leonard T. Capell, *Chairman*) with the minor modifications incorporated in the text below and also the comments following specific rules. These comments of the two inorganic nomenclature committees—together with the comments on Section 7 by the Subcommittee on Coordination Compounds (Fred Basolo, *Chairman*, and Daryle H. Busch, *Acting Chairman* at the September meeting) of the Committee on Nomenclature of the Division of Inorganic Chemistry of the American Chemical Society—are made in a spirit not of criticism but of helpfulness and with a desire to further the general use of these Rules in the United States.

The comments following specific nomenclature rules also are in smaller type for the sake of readier recognition as such, and are preceded by the symbol ◆.

Subcommittee on
Nomenclature of Inorganic
Chemistry, Division of
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Technology, National
Research Council

Miss Janet D. Scott, *Chairman*
Dr. Fred Basolo
Dr. W. C. Fernelius
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1. ELEMENTS

1.1. Names and Symbols of the Elements

1.11.—The elements should have the symbols given in the following table (Table I). It is desirable that the names should differ as little as possible among the different languages, but as complete uniformity is hard to achieve, separate lists have been drawn up in English and in French. The English list only is reproduced here.

TABLE I

ELEMENTS

Name	Symbol	Atomic number	Name	Symbol	Atomic number	Name	Symbol	Atomic number
Actinium	Ac	89	Gold (Aurum)	Au	79	Praseodymium	Pr	59
Aluminum	Al	13	Hafnium	Hf	72	Promethium	Pm	61
Americium	Am	95	Helium	He	2	Protactinium	Pa	91
Antimony	Sb	51	Holmium	Ho	67	Radium	Ra	88
Argon	Ar	18	Hydrogen	H	1	Radon	Rn	86
Arsenic	As	33	Indium	In	49	Rhenium	Re	75
Astatine	At	85	Iodine	I	53	Rhodium	Rh	45
Barium	Ba	56	Iridium	Ir	77	Rubidium	Rb	37
Berkelium	Bk	97	Iron (Ferrum)	Fe	26	Ruthenium	Ru	44
Beryllium	Be	4	Krypton	Kr	36	Samarium	Sm	62
Bismuth	Bi	83	Lanthanum	La	57	Scandium	Sc	21
Boron	B	5	Lead (Plumbum)	Pb	82	Selenium	Se	34
Bromine	Br	35	Lithium	Li	3	Silicon	Si	14
Cadmium	Cd	48	Lutetium	Lu	71	Silver (Argentum)	Ag	47
Calcium	Ca	20	Magnesium	Mg	12	Sodium	Na	11
Californium	Cf	98	Manganese	Mn	25	Strontium	Sr	38
Carbon	C	6	Mendelevium	Md	101	Sulfur	S	16
Cerium	Ce	58	Mercury	Hg	80	Tantalum	Ta	73
Cesium	Cs	55	Molybdenum	Mo	42	Technetium	Tc	43
Chlorine	Cl	17	Neodymium	Nd	60	Tellurium	Te	52
Chromium	Cr	24	Neon	Ne	10	Terbium	Tb	65
Cobalt	Co	27	Neptunium	Np	93	Thallium	Tl	81
Copper (Cuprum)	Cu	29	Nickel	Ni	28	Thorium	Th	90
Curium	Cm	96	Niobium	Nb	41	Thulium	Tm	69
Dysprosium	Dy	66	Nitrogen	N	7	Tin (Stannum)	Sn	50
Einsteinium	Es	99	Nobelium	No	102	Titanium	Ti	22
Erbium	Er	68	Osmium	Os	76	Tungsten (Wolfram)	W	74
Europium	Eu	63	Oxygen	O	8	Uranium	U	92
Fermium	Fm	100	Palladium	Pd	46	Vanadium	V	23
Fluorine	F	9	Phosphorus	P	15	Xenon	Xe	54
Francium	Fr	87	Platinum	Pt	78	Ytterbium	Yb	70
Gadolinium	Gd	64	Plutonium	Pu	94	Yttrium	Y	39
Gallium	Ga	31	Polonium	Po	84	Zinc	Zn	30
Germanium	Ge	32	Potassium	K	19	Zirconium	Zr	40

◆ The committees reaffirm the name niobium for element 41 in spite of the fact that many in the United States, particularly outside of chemical circles, still retain the name columbium.

1.12.—The names placed in parentheses (after the trivial names) in the list in Table I shall always be used when forming names derived from those of the elements, *e.g.*, aurate, ferrate, wolframate and not goldate, ironate, tungstate.

For some compounds of sulfur, nitrogen, and antimony, derivatives of the Greek name θεῖον, the French name *azote*, and the Latin name *stibium*, respectively, are used.

Although the name nickel agrees with the chemical symbol, it is essentially a trivial name and is spelled so differently in various languages (niquel, nikkel, *etc.*) that it is recommended that names of derivatives be formed from the Latin name *niccolum*, *e.g.*, niccolate instead of nickelate. The name mercury should be used as the root name also in languages where the element has another name (mercurate, *not* hydrargyrate).

In the cases in which different names have been used, the Commission has selected one based upon considerations of prevailing usage and practicability. It should be emphasized that their selection carries no implication regarding priority of discovery.

◆ Tungstate and nickelate are both so well established in American practice that the committees object to changing them to wolframate and niccolate.

1.13.—Any new metallic elements should be given names ending in -ium. Molybdenum and a few other elements have long been spelled without an "i" in most languages, and the Commission hesitates to insert it.

1.14.—All new elements shall have two-letter symbols.

1.15.—All isotopes of an element should have the same name. For hydrogen the isotope names protium, deuterium, and tritium may be retained, but it is undesirable to assign isotopic names instead of numbers to other elements. They should be designated by mass numbers as, for example, "oxygen-18."

◆ The list in 3.21 implies that D is an acceptable symbol for deuterium, whereas ^{2}H is used in 1.32. It is recommended that D and T be allowed for deuterium and tritium, respectively. *Cf.* comments made at 1.31, 1.32.

1.2 Names for Groups of Elements and their Subdivisions

1.21.—The use of the collective names: halogens (F, Cl, Br, I, and At), chalcogens (O, S, Se, Te, and Po), and halides and chalcogenides for their compounds, alkali metals (Li to Fr), alkaline earth metals (Ca to Ra), and inert gases may be continued. The name rare earth metals may be used for the elements Sc, Y, and La to Lu inclusive; the name lanthanum series for the elements no. 57–71 (La to Lu inclusive), and the name lanthanides for the elements 58–71 (Ce to Lu inclusive) are recommended. Elements no. 89 (Ac) to 103 form the actinium series, and the name actinides is reserved for the elements in which the 5*f* shell is being filled. The name transuranium elements is also approved for the elements following uranium.

◆ The collective term halogenides used in the Rules has been replaced in this version by halides, which is almost universally used in English and is unambiguous.

The inclusion of Sc with the rare earths is questioned by some. No need is seen for the terms lanthanum series and actinium series, particularly since the latter term is used for a radioactive series. The use of a collective term for elements 58–71 is approved, although it is suggested that lanthan*oid* is preferable to lanthan*ide* because of the use of -ide for binary compounds; similarly, actin*oid* is preferable to actin*ide*. Definition by means of atomic numbers is recommended in both cases rather than on the basis of interpretation (*e.g.*, filling of 5*f* shells).

1.22.—The word metalloid should not be used to denote nonmetals.

1.3 Indication of Mass, Charge, etc., on Atomic Symbols

1.31.—The mass number, atomic number, number of atoms, and ionic charge of an element may be indicated by means of four indices placed around the symbol. The positions are to be occupied thus

left upper index	mass number
left lower index	atomic number
right lower index	number of atoms
right upper index	ionic charge

Ionic charge should be indicated by A^{n+} rather than by A^{+n}.

Example: $^{32}_{16}S^{2+}_{2}$ represents a doubly ionized molecule containing two atoms of sulfur, each of which has the atomic number 16 and mass number 32.

The following is an example of an equation for a nuclear reaction

$$^{26}_{12}Mg + ^{4}_{2}He = ^{29}_{13}Al + ^{1}_{1}H$$

◆ Although the practice of American chemists and physicists in general has been to put the mass number at the upper right of the symbol, the committees recognize the advantage of putting it at the upper left so that the upper right is available for the ionic charge as needed.

1.32.—Isotopically labeled compounds may be described by adding to the name of the compounds the symbol of the isotope in parentheses.

Examples:

$^{32}PCl_3$ phosphorus(^{32}P) trichloride
(spoken: phosphorus-32 trichloride)

$H^{36}Cl$ hydrogen chloride(^{36}Cl)
(spoken: hydrogen chloride-36)

$^{15}NH_3$ ammonia(^{15}N)
(spoken: ammonia nitrogen-15)

The position of the labeled atom may be indicated by placing the isotope symbol immediately after the locant (name of the group concerned).

Example: $^{2}H_2{}^{35}SO_4$ sulfuric(^{35}S) acid(^{2}H)

If this method gives names which are ambiguous or difficult to pronounce, the whole group containing the labeled atom may be indicated.

Examples:

$HOSO_2{}^{35}SH$	thiosulfuric(^{35}SH) acid
$^{15}NO_2NH_2$	nitramide($^{15}NO_2$), not nitr(^{15}N)amide
$NO_2{}^{15}NH_2$	nitramide($^{15}NH_2$)
$HO_3S^{18}O{-}^{18}OSO_3H$	peroxo($^{18}O_2$)disulfuric acid

◆ Since IUPAC rules for labeling organic compounds are not yet available, *Chemical Abstracts* uses the modified Boughton system for deuterium and tritium compounds. For other labeled compounds the symbol in italics for the isotope introduced is attached by a hyphen to the end of the part of the name which is modified.

1.4. Allotropes

If systematic names for gaseous and liquid modifications are required, they should be based on the size of the molecule, which can be indicated by Greek numerical prefixes (listed in **2.251**). If the number of atoms is large and unknown, the prefix poly may be used. To indicate ring and chain structures the prefixes cyclo and catena may be used.

Examples:

Symbol	Trivial Name	Systematic Name
H	atomic hydrogen	monohydrogen
O_2	(common) oxygen	dioxygen
O_3	ozone	trioxygen
P_4	white phosphorus (yellow phosphorus)	tetraphosphorus
S_8	λ-sulfur	cycloöctasulfur or octasulfur
S_n	μ-sulfur	catenapolysulfur or polysulfur

For the nomenclature of solid allotropic forms the rules in Section **8** may be applied.

◆ The use of prefixes to indicate ring and chain structures is favored by the committees, but it should be pointed out that ino (not catena) has been used by mineralogists for indicating chain structures in silicates, along with cyclo and other prefixes (neso, phyllo, tecto, soro) denoting structure, all used without italics or hyphens (*e.g.*, inosilicates). *Cf.* use of catena in 7.42 for chains of alternating, not self-linking, atoms.

2. FORMULAS AND NAMES OF COMPOUNDS IN GENERAL

Many chemical compounds are essentially binary in nature and can be regarded as combinations of ions or radicals; others may be treated as such for the purpose of nomenclature.

Some chemists have expressed the opinion that the name of a compound should indicate whether it is ionic or covalent. Such a distinction is made in some languages (*e.g.*, in German: Natriumchlorid *but* Chlorwasserstoff), but it has not been made consistently, and indeed it seems impossible to introduce this distinction into a consistent system of nomenclature, because the line of demarcation between these two categories is not sharp. In these rules a system of nomenclature has been built on the basis of the endings -ide and -ate, and it should be emphasized that these are intended to be applied both to ionic and covalent compounds. If it is desired to avoid such endings for neutral molecules, names can be given as coördination compounds in accordance with **2.24** and Section **7**.

2.1. Formulas

2.11.—Formulas provide the simplest and clearest method of designating inorganic compounds. They are of particular importance in chemical equations and in descriptions of chemical procedure. However, their general use in text is not recommended, although in some cases a formula, on account of its compactness, may be preferable to a cumbersome and awkward name.

2.12.—The *empirical formula* is formed by juxtaposition of the atomic symbols to give the *simplest possible* formula expressing the stoichiometric composition of the compound in question. The empirical formula may be supplemented by indication of the crystal structure—see Section 8.

2.13.—For compounds consisting of discrete molecules the *molecular formula*, *i.e.*, a formula corresponding with the correct molecular weight of the compound, should be used, *e.g.*, S_2Cl_2 and $H_4P_2O_6$ and not SCl and H_2PO_3. When the molecular weight varies with temperature, *etc.*, the simplest possible formula generally may be chosen, *e.g.*, S, P, and NO_2 instead of S_8, P_4, and N_2O_4, unless it is desirable to indicate the molecular complexity.

2.14.—In the *structural formula* the sequence and spatial arrangement of the atoms in a molecule are indicated.

2.15.—In formulas the *electropositive constituent* (cation) should always be placed first, *e.g.*, KCl, $CaSO_4$.

This also applies in Romance languages even though the electropositive constituent is placed last in the *name*, *e.g.*, KCl, chlorure de potassium.

If the compound contains more than one electropositive or more than one electronegative constituent, their sequence is determined by Rules **6.32** and **6.33**.

2.16.—In the case of binary compounds between nonmetals that constituent should be placed first which appears earlier in the sequence: B, Si, C, Sb, As, P, N, H, Te, Se, S, At, I, Br, Cl, O, F.

Examples: NH_3, H_2S, N_4S_4, S_2Cl_2, Cl_2O, OF_2

◆ Because N_4S_4 is definitely a nitride, not a sulfide, the committees prefer to write the formula S_4N_4, name it sulfur nitride, and cite it as an exception rather than as an example.

2.161.—For compounds containing three or more elements, however, the sequence should in general follow the order in which the atoms are actually bound in the molecule or ion, *e.g.*, NCS^-, not CNS^-, HOCN (cyanic acid), and HONC (fulminic acid).

Although formulas such as HNO_3, $HClO_4$, H_2SO_4, do not agree with this rule and HNO_3 does not even follow the main rule in **2.16**, the Commission does not at this time wish to break the old custom of putting the central atom immediately after the hydrogen atom in such cases (*cf.* Section 5). The formula for hypochlorous acid may be written HOCl or HClO.

2.17.—In intermetallic compounds the constituents should be placed in the order

Fr, Cs, Rb, K, Na, Li
Ra, Ba, Sr, Ca, Mg, Be
103, No, Md, Fm, Es, Cf, Bk, Cm, Am, Pu, Np, U, Pa, Th, Ac, Lu–La, Y, Sc
Hf, Zr, Ti
Ta, Nb, V
W, Mo, Cr
Re, Tc, Mn
Pt, Ir, Os, Pd, Rh, Ru, Ni, Co, Fe
Au, Ag, Cu
Hg, Cd, Zn
Tl, In, Ga, Al
Pb, Sn, Ge
Bi, Sb
Po
Nonmetals (except Sb) in the order given in **2.16**.

Deviations from this order may be allowed, *e.g.*, when compounds with analogous structures are compared (AgZn and AgMg).

2.18.—The number of identical atoms or atomic groups in a formula is indicated by means of Arabic numerals, placed below and to the right of the symbol or symbols in parentheses ( ) or brackets [ ] to which they refer. Water of crystallization and similar loosely bound molecules, however, are designated by means of Arabic numerals before their formulas.

Examples: $CaCl_2$ not $CaCl^2$
$[Co(NH_3)_6]Cl_3$ not $[Co6NH_3]Cl_3$
$[Co(NH_3)_6]_2(SO_4)_3$
$Na_2SO_4.10H_2O$

2.19.—The prefixes *cis*, *trans*, *sym*, *asym* may be used in their usual senses. The prefixes may be connected with the formula by a hyphen and it is recommended that they be italicized.

Example: *cis*-$[PtCl_2(NH_3)_2]$

2.2. Systematic Names

Systematic names of compounds are formed by indicating the constituents and their proportions according to the following rules. (For the order of the constituents see also the later sections.)

2.21.—The name of the *electropositive constituent* (or that treated as such according to **2.16**) will not be modified (see, however, **2.2531**).

In Germanic languages the electropositive constituent is placed first, but in Romance languages it is customary to place the electronegative constituent first.

2.22.—If the *electronegative constituent* is monatomic its name is modified to end in -ide. For binary compounds of the nonmetals the name of the element standing later in the sequence in **2.16** is modified to end in -ide.

Examples: Sodium chloride, calcium sulfide, lithium nitride, arsenic selenide, calcium phosphides, nickel arsenide, aluminum borides, iron carbides, boron hydrides, phosphorus hydrides, hydrogen chloride, hydrogen sulfide, silicon carbide, carbon disulfide, sulfur hexafluoride, chlorine dioxide, oxygen difluoride.

Certain polyatomic groups are also given the ending -ide—see **3.22**.

In the Romance languages the endings -ure, -uro, and -eto are used instead of -ide. In some languages the word *oxyde* is used, whereas the ending -ide is used in the names of other binary compounds; it is recommended that the ending -ide be universally adopted in these languages.

◆ Nitrogen sulfide has been taken out of the examples. *Cf.* comment at 2.16.

2.23.—If the electronegative constituent is polyatomic it should be designated by the termination -ate.

In certain exceptional cases the terminations -ide and -ite are used—see **3.22**.

2.24.—In inorganic compounds it is generally possible in a polyatomic group to indicate a *characteristic atom* (as in ClO^-) or a *central atom* (as in ICl_4^-). Such a polyatomic group is designated a *complex*, and the atoms, radicals, or molecules bound to the characteristic or central atom are termed *ligands*.

In this case the name of a negatively charged complex should be formed from the name of the characteristic or central element (as indicated in **1.12**) modified to end in -ate.

Anionic ligands are indicated by the termination -o. Further details concerning the designation of ligands, the definition of "central atom," *etc.*, appear in Section **7**.

Although the terms sulfate, phosphate, *etc.*, were originally the names of the anions of particular oxo acids, the names sulfate, phosphate, *etc.*, should now designate quite generally a negative group containing sulfur or phosphorus, respectively, as the central atom, irrespective of its oxidation state (the designation of the oxidation state is discussed in later rules) and the number and nature of the ligands. The complex is indicated by brackets [ ], but this is not always necessary.

Examples:

$Na_2[SO_4]$	sodium tetraoxosulfate
$Na_2[SO_3]$	sodium trioxosulfate
$Na_2[S_2O_3]$	sodium trioxothiosulfate
$Na[SO_3F]$	sodium trioxofluorosulfate
$Na_3[PO_4]$	sodium tetraoxophosphate
$Na_3[PS_4]$	sodium tetrathiophosphate
$Na[PCl_6]$	sodium hexachlorophosphate
$K[PO_2F_2]$	potassium dioxodifluorophosphate
$K[POCl_2(NH)]$	potassium oxodichloroimidophosphate

In many cases these names may be abbreviated, *e.g.*, sodium sulfate, sodium thiosulfate (see **2.26**), and in other cases trivial names may be used (*cf.* **2.3**, **3.224**, and Section **5**). It should be pointed out, however, that the principle is quite generally applicable, to compounds containing organic ligands also, and its use is recommended in all cases where trivial names do not exist.

The coördination principle applied in this rule may also be applied to complexes which are positive or neutral (*cf.* **3.1** and Section **7**). However, neutral complexes which are as a rule considered as binary compounds are given names according to **2.22**, **2.16**. Thus, SO_3, sulfur trioxide, not trioxosulfur.

◆ In the examples it would seem that full coördination-type names should be given, *e.g.*, either sodium tetraoxosulfate (VI) or disodium tetraoxosulfate. *Cf.* 7.32 and comment at 7.312.

2.25.—Indication of the Proportions of the Constituents.

2.251.—The *stoichiometric proportions* may be denoted by means of Greek numerical prefixes (mono, di, tri, tetra, penta, hexa, hepta, octa, ennea, deca, hendeca, and dodeca) preceding without hyphen the names of the elements to which they refer. It may be necessary in some languages to supplement these numerals with hemi ($^1/_2$) and the Latin sesqui ($^3/_2$).

The prefix mono may generally be omitted. Beyond 12, Greek prefixes are replaced by Arabic numerals (with or without hyphen according to the custom of the language), because they are more readily understood.

This system is applicable to all types of compounds and is especially suitable for binary compounds of the nonmetals.

When it is required to indicate the number of entire groups of atoms, particularly when the name includes a numerical prefix with a different significance, the multiplicative numerals (Latin bis, Greek tris, tetrakis, *etc.*) are used and the whole group to which they refer may be placed in parentheses if necessary.

Examples:

N_2O	dinitrogen oxide
NO_2	nitrogen dioxide
N_2O_4	dinitrogen tetraoxide
N_2S_5	dinitrogen pentasulfide
S_2Cl_2	disulfur dichloride
Fe_3O_4	triiron tetraoxide
U_3O_8	triuranium octaoxide
MnO_2	manganese dioxide
$Ca_3[PO_4]_2$	tricalcium diorthophosphate
$Ca[PCl_6]_2$	calcium bis(hexachlorophosphate)

In indexes it may be convenient to italicize a numerical prefix at the beginning of the name and connect it to the rest of the name with a hyphen, but this is not desirable in text, *e.g.*, *tri*-Uranium octaoxide.

Since the degree of polymerization of many substances varies with temperature, state of aggregation, *etc.*, the name to be used should normally be based upon the simplest possible formula of the substance except when it is required specifically to draw attention to the degree of polymerization.

Example: The name nitrogen dioxide may be used for the equilibrium mixture of NO_2 and N_2O_4. Dinitrogen tetraoxide means specifically N_2O_4.

◆ In accordance with the organic nomenclature rules and well-established practice, it is recommended that "or Latin" be inserted between "Greek" and "numerical prefixes" in the first sentence and that "nona" replace "ennea," and "undeca" replace "hendeca."

Extreme caution is advised in the omission of numerical prefixes, including mono (*cf.* second set of examples in 5.23), because of the frequent use of names such as chloroplatinate (*cf.* 2.26 and the last sentence in 5.24).

2.252.—The proportions of the constituents also may be indicated indirectly by *Stock's system*, that is, by Roman numerals representing the oxidation number or stoichiometric valence of the element, placed in parentheses immediately following the name. For zero the Arabic 0 will be used. When used in conjunction with symbols the Roman numeral may be placed above and to the right.

The Stock notation can be applied to both cations and anions, but preferably should *not* be applied to compounds between nonmetals.

In employing the Stock notation, use of the Latin names of the elements (or Latin roots) is considered advantageous.

Examples:

$FeCl_2$	iron(II) chloride or ferrum(II) chloride
$FeCl_3$	iron(III) chloride or ferrum(III) chloride
MnO_2	manganese(IV) oxide
BaO_2	barium(II) peroxide
$Pb^{II}_2Pb^{IV}O_4$	dilead(II) lead(IV) oxide or trilead tetraoxide
$K_4[Ni(CN)_4]$	potassium tetracyanonicollate(0)
$K_4[Fe(CN)_6]$	potassium hexacyanoferrate(II)
$Na_2[Fe(CO)_4]$	sodium tetracarbonylferrate(−II)

◆ While the committees favor the extended use of the Stock notation, they suggest that in some cases the system of Ewens and Bassett (designation of the aggregate charge of a complex ion by an Arabic numeral in parentheses following the name, similar to the use as superior notations with formulas) is advantageous and should be allowed as an alternate (*cf.* 3.17 and comment at 7.323). Mixed use of the two systems, while not desirable in any one context, does not affect indexing and should not lead to confusion. See comment at 1.12.

2.253.—The following systems are in use but are not recommended:

2.2531.—The system of indicating valence by means of the suffixes *-ous* and *-ic* added to the root of the name of the cation may be retained for elements exhibiting not more than two valences.

2.2532.—"*Functional*" nomenclature (such as "nitric anhydride" for N_2O_5) is not recommended apart from the name *acid* to designate the acid function (Section **5**).

◆ Apparently there is no objection to acid anhydride as a class name (*cf.* 5.32). Other functional derivatives of acids are named as such in the Rules (5.3).

2.26.—In systematic names it is not always necessary to indicate stoichiometric proportions. In many instances it is permissible to omit the numbers of atoms, oxidation numbers, *etc.*, when they are not required in the particular circumstances. For instance, these indications are not generally necessary with elements of essentially constant valence.

Examples:

- sodium sulfate instead of sodium tetraoxosulfate
- aluminum sulfate instead of aluminum(III) sulfate
- potassium chloroplatinate(IV) instead of potassium hexachloroplatinate(IV)
- potassium cyanoferrate(III) instead of potassium hexacyanoferrate(III)
- phosphorus pentaoxide instead of diphosphorus pentaoxide

2.3. Trivial Names

Certain well-established trivial names for oxo acids (Section **5**) and for hydrogen compounds (water, ammonia, hydrazine) are still acceptable. For some other hydrogen compounds these names are approved

B_2H_6	diborane		
SiH_4	silane	Si_2H_6	disilane, *etc.*
PH_3	phosphine	P_2H_4	diphosphine
AsH_3	arsine	As_2H_4	diarsine
SbH_3	stibine		

In some languages names of the type "Chlorwasserstoff" are in use and may be retained if national nomenclature committees so wish.

Purely trivial names, free from false scientific implications, such as soda, Chile saltpeter, quicklime, are harmless in industrial and popular literature; but old incorrect scientific names such as sulfate of magnesia, Natronhydrat, sodium muriate, carbonate of lime, should be avoided under all circumstances, and they should be eliminated from technical and patent literature.

◆ For BH_3 (omitted in the Rules) borane rather than the previously used borine has been recommended by the Advisory Committee on the Nomenclature of Organic Boron Compounds of the ACS in a report not yet published.

Because soda is an ambiguous term, it is suggested that it be replaced by soda ash.

3. NAMES FOR IONS AND RADICALS

3.1. Cations

3.11.—Monatomic cations should be named like the corresponding element, without change or suffix, except as provided by **2.2531.**

Examples:

Cu^+	the copper(I) ion
Cu^{2+}	the copper(II) ion
I^+	the iodine cation

◆ For I^+, iodide(I) cation is more consistent with recommended practice. *Cf.* 3.21.

3.12.—The preceding principle should apply also to polyatomic cations corresponding to radicals for which special names are given in **3.32**, *i.e.*, these names should be used without change or suffix.

Examples:

NO^+	the nitrosyl cation
NO_2^+	the nitryl cation

◆ Polyatomic here and in 3.13, 3.14, 3.223, 3.32, and 5.2 seems to be limited to more than one *kind* of atom, and hence heteratomic would be a more precise term. It is agreed that nitryl and not nitronium should be used in all cases (*cf.* 3.151).

3.13.—Polyatomic cations formed from monatomic cations by the addition of other ions or neutral atoms or molecules (ligands) will be regarded as complex and will be named according to the rules given in Section **7.**

Examples:

$[Al(H_2O)_6]^{3+}$	the hexaaquoaluminum ion
$[CoCl(NH_3)_5]^{2+}$	the chloropentamminecobalt ion

For some important polyatomic cations which fall in this section, radical names given in **3.32** may be used alternatively, *e.g.*, for UO_2^{2+} the name uranyl(VI) ion in place of dioxouranium(VI) ion.

3.14.—Names for polyatomic cations derived by addition of protons to monatomic anions are formed by adding the ending -onium to the root of the name of the anion element.

Examples: phosphonium, arsonium, stibonium, oxonium, sulfonium, selenonium, telluronium, and iodonium ions.

Organic ions derived by substitution in these parent cations should be named as such, whether the parent itself is a known compound or not: for example $(CH_3)_4Sb^+$, the tetramethylstibonium ion.

The ion H_3O^+, which is in fact the monohydrated proton, is to be known as the oxonium ion when it is believed to have this constitution, as for example in $H_3O^+ClO_4^-$, oxonium perchlorate. The widely used term hydronium should be kept for the cases where it is wished to denote an indefinite degree of hydration of the proton, as, for example, in aqueous solution. If, however, the hydration is of no particular importance to the matter under consideration, the simpler term hydrogen ion may be used. The latter also may be used for the indefinitely solvated proton in nonaqueous solvents; but definite ions such as $CH_3OH_2^+$ and $(CH_3)_2OH^+$ should be named as derivatives of the oxonium ion, *i.e.*, as methyl- and dimethyloxonium ions, respectively.

◆ The committees concur in oxonium for the ion H_3O^+, but see little reason for encouraging retention of the term hydronium ion because hydrogen ion adequately designates an indeterminate degree of hydration.

3.15.—Ions from Nitrogen Bases.

3.151.—The name ammonium for the ion NH_4^+ does not conform to **3.14**, but should be retained. This decision does *not* release the word nitronium for other uses: this would lead to inconsistencies when the rules are applied to other elements.

3.152.—Substituted ammonium ions derived from nitrogen bases with names ending in -amine will receive names formed by changing -amine to -ammonium. For example, $HONH_3^+$, the hydroxylammonium ion.

3.153.—When the nitrogen base is known by a name ending otherwise than in -amine, the cation name is to be formed by adding the ending -ium to the name of the base (if necessary omitting a final -e or other vowel).

Examples: hydrazinium, anilinium, glycinium, pyridinium, guanidinium, imidazolium.

The names uronium and thiouronium, though inconsistent with this rule, may be retained.

3.16.—Cations formed by adding protons to nonnitrogenous bases may also be given names formed by adding -ium to the name of the compound to which the proton is added.

Examples: dioxanium, acetonium.

In the case of cations formed by adding protons to acids, however, their names are to be formed by adding the word acidium to the name of the corresponding anion, and not that of the acid itself. For example, $H_2NO_3^+$, the nitrate acidium ion; $H_2NO_2^+$, the nitrite acidium ion; and $CH_3COOH_2^+$, the acetate acidium ion. Note, however, that when the anion of the acid is monatomic **3.14** will apply; for example, FH_2^+ is the fluoronium ion.

◆ In accord with present practice, nitric acidium ion, *etc.*, are preferred to nitrate acidium ion, *etc.* $CH_3COOH_2^+$ is organic.

3.17.—Where more than one ion is derived from one base, as, for example, $N_2H_5^+$ and $N_2H_6^{2+}$, their charges may be indicated in their names as the hydrazinium(1+) and the hydrazinium(2+) ion, respectively.

◆ *Cf.* comment at 2.252 and the use of Stock notation with ions or radicals in 3.13 and 3.32.

3.2. Anions

3.21.—The names for monatomic anions shall consist of the name (sometimes abbreviated) of the element, with the termination -ide. Thus

H^-	hydride ion	N^{3-}	nitride ion
D^-	deuteride ion	P^{3-}	phosphide ion
F^-	fluoride ion	As^{3-}	arsenide ion
Cl^-	chloride ion	Sb^{3-}	antimonide ion
Br^-	bromide ion	C^{4-}	carbide ion
I^-	iodide ion	Si^{4-}	silicide ion
O^{2-}	oxide ion	B^{3-}	boride ion
S^{2-}	sulfide ion		
Se^{2-}	selenide ion		
Te^{2-}	telluride ion		

Expressions of the type "chlorine ion" are used particularly in connection with crystal structure work and spectroscopy; the Commission recommends that whenever the charge corresponds with that indicated above, the termination -ide should be used.

◆ *Cf.* comments at 1.15 and 1.32 regarding ^2H and D.

3.22.—Polyatomic Anions.

3.221.—Certain polyatomic anions have names ending in -ide. These are

OH^-	hydroxide ion	N_3^-	azide ion
O_2^{2-}	peroxide ion	NH^{2-}	imide ion
O_2^-	hyperoxide ion	NH_2^-	amide ion
O_3^-	ozonide ion	$NHOH^-$	hydroxylamide ion
S_2^{2-}	disulfide ion		
I_3^-	triiodide ion	$N_2H_3^-$	hydrazide ion
HF_2^-	hydrogen difluoride ion	CN^-	cyanide ion
		C_2^{2-}	acetylide ion

Names for other polysulfide, polyhalide, *etc.*, ions may be formed in analogous manner. The OH^- ion should not be called the hydroxyl ion. The name hydroxyl is reserved for the OH group when neutral or positively charged, whether free or as a substituent (*cf.* **3.12** and **3.32**).

◆ Superoxide is well established in English for O_2^- and no advantage is seen in changing to hyperoxide.

3.222.—Ions such as SH^- and O_2H^- will be called the hydrogen sulfide ion and the hydrogen peroxide ion, respectively. This agrees with **6.2**, and names such as hydrosulfide are not needed.

◆ *Cf.* comment at 6.2. All "fused" names (as hydrogensulfide here and methylisocyanide in 5.33) in the original version have been written as two words in this version. For a rule on the written form of the names of compounds see *J. Chem. Education*, **8**, 1336–8 (1931).

3.223.—The names for other polyatomic anions shall consist of the name of the central atom with the termination -ate, which is used quite generally for complex anions. Atoms and groups attached to the central atom shall generally be treated as ligands in a complex (*cf.* **2.24** and Section **7**) as, for example, $[Sb(OH)_6]^-$, the hexahydroxoantimonate(V) ion.

This applies also when the exact composition of the anion is not known; *e.g.*, by solution of aluminum hydroxide or zinc hydroxide in sodium hydroxide, aluminate and zincate ions are formed.

3.224.—It is quite practicable to treat oxygen in the same manner as other ligands (**2.24**), but it has long been customary to ignore the name of this element altogether in anions and to indicate its presence and proportion by means of a series of prefixes (hypo-, per-, *etc.*, see Section **5**) and sometimes also by the suffix -ite in place of -ate.

The termination -ite has been used to denote a lower oxidation state and may be retained in trivial names in these cases

NO_2^-	nitrite
$N_2O_2^{2-}$	hyponitrite
NOO_2^-	peroxonitrite
PHO_3^{2-}	phosphite
$P_2H_2O_5^{2-}$	diphosphite (pyrophosphite)
$PH_2O_2^-$	hypophosphite
AsO_3^{3-}	arsenite
SO_3^{2-}	sulfite
$S_2O_5^{2-}$	disulfite (pyrosulfite)
$S_2O_4^{2-}$	dithionite
$S_2O_2^{2-}$	thiosulfite
SeO_3^{2-}	selenite
ClO_2^-	chlorite
ClO^-	hypochlorite

(and correspondingly for the other halogens)

The Commission does not recommend the use of any such names other than those listed. A number of other names ending in -ite have been used, *e.g.*, antimonite, tellurite, stannite, plumbite, ferrite, manganite, but in many cases such compounds are known in the solid state to be double oxides and are to be treated as such (*cf.* **6.5**), *e.g.*, $Cu(CrO_2)_2$ copper(II) chromium(III) oxide, not copper chromite. Where there is reason to believe that a definite salt with a discrete anion exists, the name is formed in accordance with **2.24**. By dissolving, for example, Sb_2O_3, SnO, or PbO in sodium hydroxide an antimonate(III), a stannate(II), or a plumbate(II) is formed in the solution.

Concerning the use of prefixes hypo-, per-, *etc.*, see the list of acids (table in **5.214**). For all new compounds and even for the less common ones listed in the table in **3.224** or derived from the acids listed in the table in **5.214**, it is preferable to use the system given in **2.24** and in Sections **5** and **7**.

◆ For phosphite names see comment at 6.2.

3.3. Radicals

3.31.—A radical is here regarded as a group of atoms which occurs repeatedly in a number of different compounds. Sometimes the same radical fulfils different functions in different cases, and accordingly different names often have been assigned to the same group. The Commission considers it desirable to reduce this diversity and recommends that formulas or systematic names be used to denote all new radicals, instead of introducing new trivial names. The list of names for ions and radicals on page 5543 gives an extensive selection of radical names at present in use in inorganic chemistry.

◆ The list of names for ions and radicals following the Rules is very useful and can be made more so by additions (as of dithio, nitrilo, and azido in the last column) and by greater attempt at uniformity with organic usage. Some of the terms (as nitride and amide) listed as anions are used also of covalent compounds. A single atom may function like a radical as defined above and may be named similarly, as chloro and oxo.

3.32.—Certain radicals containing oxygen or other chalcogens have special names ending in -yl, and the Commission approves the provisional retention of

HO	hydroxyl
CO	carbonyl
NO	nitrosyl
NO_2	nitryl[1]
PO	phosphoryl
VO	vanadyl
SO	sulfinyl (thionyl)
SO_2	sulfonyl (sulfuryl)
S_2O_5	pyrosulfuryl
SeO	seleninyl
SeO_2	selenonyl
CrO_2	chromyl
UO_2	uranyl
NpO_2	neptunyl
PuO_2	plutonyl (similarly for other actinide elements)
ClO	chlorosyl
ClO_2	chloryl
ClO_3	perchloryl (and similarly for other halogens)

[1] The name nitroxyl should not be used for this group since the name nitroxylic acid has been used for H_4NO_3. Although the word nitryl is firmly established in English, nitroyl may be a better model for many other languages.

Names such as the above should be used only to designate compounds containing these discrete groups. The use of thionyl and sulfuryl should be restricted to the halides. Names such as bismuthyl and antimonyl are not approved because the compounds do not contain BiO and SbO groups, respectively; such compounds are to be designated as oxide halides (**6.4**).

Radicals analogous to the above containing other chalcogens in place of oxygen are named by adding the prefixes thio-, seleno-, *etc.*

Examples:

PS	thiophosphoryl	CSe	selenocarbonyl

In cases where radicals may have different valences, the oxidation number of the characteristic element should be indicated by means of the Stock notation. For example, the uranyl group UO_2 may refer either to the ion UO_2^{2+} or to the ion UO_2^+; these can be distinguished as uranyl(VI) and uranyl(V), respectively. In like manner, VO may be vanadyl(V), vanadyl(IV), and vanadyl(III).

These polyatomic radicals always are treated as forming the positive part of the compound.

Examples:

$COCl_2$	carbonyl chloride
NOS	nitrosyl sulfide
PON	phosphoryl nitride
$PSCl_3$	thiophosphoryl chloride
POCl	phosphoryl(III) chloride
$NO_2HS_2O_7$	nitryl hydrogen disulfate
S_2O_5ClF	pyrosulfuryl chloride fluoride
$SO_2(N_3)_2$	sulfonyl azide
SO_2NH	sulfonyl imide
IO_2F	iodyl fluoride

By using the same radical names regardless of unknown or controversial polarity relationships, names can be formed without entering into any controversy. Thus, for example, the compounds NOCl and $NOClO_4$ are quite unambiguously denoted by the names nitrosyl chloride and nitrosyl perchlorate, respectively.

◆ Caution is urged in the use of some of these radical names: Vanadyl, for example, has been used for VO_2 as well as for VO (*cf.* also the naming of $VOSO_4$ in 6.42). Most of these radical names (except hydroxyl and thionyl) can be regarded as derived from the names of acids which have lost all of their hydroxyls (analogous to -yl or -oyl organic acid radical names) by the use of -yl and -osyl for radicals from -ic and -ous acids, respectively; this is implied in the footnote about nitroxyl. The use of the Stock notation in only one example (phosphoryl(III) chloride) seems confusing. It might be clearer to indicate stoichiometric proportions, *e.g.*, phosphoryl (mono)chloride, thiophosphoryl trichloride (*cf.*

phosphoryl triamide in 5.34) or to use phosphorosyl for phosphoryl(III).

The restriction of the use of thionyl and sulfuryl to the halides was agreed upon at a joint meeting of the inorganic and organic nomenclature commissions of the IUPAC in 1951.

3.33.—It should be noted that the same radical may have different names in inorganic and organic chemistry. To draw attention to such differences the prefix names of radicals as substituents in organic compounds have been listed together with the inorganic names in the list of names printed at the end of the Rules. Names of purely organic compounds, of which many are important in the chemistry of coördination compounds (Section 7), should agree with the nomenclature of organic chemistry.

Organic chemical nomenclature is to a large extent based on the principle of substitution, *i.e.*, replacement of hydrogen atoms by other atoms or groups. Such "substitutive names" are extremely rare in inorganic chemistry; they are used, *e.g.*, in the following cases: NH_2Cl is called chloramine, and $NHCl_2$ dichloramine. These names may be retained in the absence of better terms. Other substitutive names (derived from "sulfonic acid" as a name for HSO_3H) are fluoro- and chlorosulfonic acid, aminosulfonic acid, iminodisulfonic acid, and nitrilotrisulfonic acid. These names should preferably be replaced by the following

FSO_3H	fluorosulfuric acid
$ClSO_3H$	chlorosulfuric acid
NH_2SO_3H	amidosulfuric acid
$NH(SO_3H)_2$	imidodisulfuric acid
$N(SO_3H)_3$	nitridotrisulfuric acid

Names such as chlorosulfuric acid and amidosulfuric acid might be considered to be substitutive names derived by substitution of *hydroxyl* groups in sulfuric acid. From a more fundamental point of view, however (see 2.24), such names are formed by adding hydroxyl, amide, imide, *etc.*, groups together with oxygen atoms to a sulfur atom, "sulfuric acid" in this connection standing as an abbreviation for "trioxosulfuric acid."

Another organic-chemical type of nomenclature, the formation of "conjunctive names," is also met in only a few cases in inorganic chemistry, *e.g.*, the hydrazine- and hydroxylaminesulfonic acids. According to the principles of inorganic chemical nomenclature these compounds should be called hydrazido- and hydroxylamidosulfuric acid.

◆ These are not true "conjunctive names" since sulfonic acid is not a compound. For the naming of partial amides *cf.* also 5.34.

4. CRYSTALLINE PHASES OF VARIABLE COMPOSITION

Isomorphous replacement, interstitial solutions, intermetallic compounds, and other nonstoichiometric compounds (berthollides)

4.1.—If an intermediate crystalline phase occurs in a two-component (or more complex) system, it may obey the law of constant composition very closely, as in the case of sodium chloride, or it may be capable of varying in composition over an appreciable range, as occurs for example with FeS. A substance showing such a variation is called a *berthollide*.

In connection with the berthollides the concept of a characteristic or ideal composition is frequently used. A unique definition of this concept seems to be lacking. In one case it may be necessary to use a definition based upon lattice geometry and in another to base it on the ratio of valence electrons to atoms. Sometimes one can state several characteristic compositions, and at other times it is impossible to say whether a phase corresponds to a characteristic composition or not.

In spite of these difficulties it seems that the concept of a characteristic composition can be used in its present undefined form for establishing a system of notation for phases of variable composition. It also seems possible to use the concept even if the characteristic composition is not included in the known homogeneity range of the phase.

4.2.—For the present, mainly formulas should be used for berthollides and solid solutions, since strictly logical names tend to become inconveniently cumbersome. The latter should be used only when unavoidable (*e.g.*, for indexing), and may be written in the style of iron(II) sulfide (iron-deficient); molybdenum dicarbide (excess carbon), or the like. Mineralogical names should be used only to designate actual minerals and not to define chemical composition; thus the name calcite refers to a particular mineral (contrasted with other minerals of similar composition) and is not a term for the chemical compound whose composition is properly expressed by the name calcium carbonate. (The mineral name may, however, be used to indicate the structure type—see 6.52.)

4.3.—A general notation for the berthollides, which can be used even when the mechanism of the variation in composition is unknown, is to put the sign $\sim$ (read as *circa*) before the formula. (In special cases it may also be printed above the formula.)

Examples: $\sim FeS$, $\overset{\sim}{CuZn}$

The direction of the deviation may be indicated when required:

$\sim FeS$ (iron-deficient); $\sim MoC_2$ (excess carbon)

4.4.—For a phase where the variable composition is solely or partially caused by replacement, atoms or atomic groups which replace each other are separated by a comma and placed together between parentheses.

If possible the formula ought to be written so that the limits of the homogeneity range are represented when one or other of the two atoms or groups is lacking. For example the symbol (Ni,Cu) denotes the complete range from pure Ni to pure Cu; likewise K(Br,Cl) comprises the range from pure KBr to pure KCl. If only part of the homogeneity range is referred to, the major constituent should be placed first.

Substitution accompanied by the appearance of vacant positions (combination of substitutional and interstitial solution) receives an analogous notation. For example, $(Li_2,Mg)Cl_2$ denotes the homogeneous phase from LiCl to $MgCl_2$ where the anion lattice structure remains the same but one vacant cation position appears for every substitution of $2Li^+$ by Mg^{2+}.

The formula $(Mg_3,Al_2)Al_6O_{12}$ represents the homogeneous phase from the spinel $MgAl_2O_4$ ($= Mg_3Al_6O_{12}$) to the spinel form of Al_2O_3 ($= Al_2Al_6O_{12}$).

The solid solutions between CaF_2 and YF_3, where cation substitution is accompanied by interstitial addition of F^-, would be represented by the formula $(Ca,YF)F_2$. It is important to note that this formula is based purely on considerations of composition, and it does not imply that YF^{2+} takes over the actual physical position of Ca^{2+}. On the same basis a notation for the plagioclases would be $(NaSi,CaAl)Si_2AlO_8$.

4.5.—A still more complete notation, which should always be used in more complex cases, may be constructed by indicating in a formula the variables that define the composition. Thus, a phase involving simple substitution may be written A_xB_{1-x}.

Examples: Ni_xCu_{1-x} and KBr_xCl_{1-x}

This shows immediately that the total number of atoms in the lattice is constant. Combined substitutional and interstitial or subtractive solution can be shown in an analogous way. The commas and parentheses called for in **4.4** are not required in this case.

For example, the homogeneous phase between LiCl and $MgCl_2$ becomes $Li_{2x}Mg_{1-x}Cl_2$ and the phase between $MgAl_2O_4$ and Al_2O_3 can be written $Mg_{3x}Al_{2(1-x)}Al_6O_{12}$, which shows that it cannot contain more Mg than that corresponding to $MgAl_2O_4$ ($x = 1$). The other examples given in **4.4** will be given the formulas $Ca_xY_{1-x}F_{3-x}$ and $Na_xCa_{1-x}Si_{2+x}Al_{2-x}O_8$. In the case of the γ-phase of the Ag–Cd system, which has the characteristic formula Ag_5Cd_8, the Ag and Cd atoms can replace one another to some extent and the notation would be $Ag_{5\pm x}Cd_{8\mp x}$.

Further examples:

$Fe_{1-x}Sb$ $Fe_{1-x}O$ $Fe_{1-x}S$ $Cu_{2-x}O$

$Na_{1-x}WO_3$ (sodium tungsten bronzes)

For $x = 0$ each of these formulas corresponds to a characteristic composition. If it is desired to show that the variable denoted by x can attain only small values, this may be done by substituting ϵ for x.

Likewise a solid solution of hydrogen in palladium can be written as PdH_x, and a phase of the composition M which has dissolved a variable amount of water can be written $M(H_2O)_x$.

When this notation is used, a particular composition can be indicated by stating the actual value of the variable x. Probably the best way of doing this is to put the value in parentheses after the general formula. For example, $Li_{4-x}Fe_{3x}Ti_{2(1-x)}O_6$ ($x = 0.35$). If it is desired to introduce the value of x into the formula itself, the mechanism of solution is more clearly understood if one writes $Li_{4-0\cdot35}Fe_{3\times0\cdot35}Ti_{2(1-0\cdot35)}O_6$ instead of $Li_{3\cdot65}Fe_{1\cdot05}Ti_{1\cdot30}O_6$.

5. ACIDS

Many of the compounds which now according to some definitions are called acids do not fall into the classical province of acids. In other parts of inorganic chemistry functional names are disappearing and it would have been most satisfactory to abolish them also for those compounds generally called acids. Names for these acids may be derived from the names of the anions as in Section **2**, *e.g.*, hydrogen sulfate instead of sulfuric acid. The nomenclature of acids has, however, a long history of established custom, and it appears impossible to systematize acid names without drastic alteration of the accepted names of many important and well-known substances.

The present rules are aimed at preserving the more useful of the older names while attempting to guide further development along directions which should allow new compounds to be named in a more systematic manner.

5.1. Binary and Pseudobinary Acids

Acids giving rise to the -ide anions defined by **3.21** and **3.221** will be named as binary and pseudobinary compounds of hydrogen, *e.g.*, hydrogen chloride, hydrogen sulfide, hydrogen cyanide.

For the compound HN_3 the name hydrogen azide is recommended in preference to hydrazoic acid.

5.2. Acids Derived from Polyatomic Anions

Acids giving rise to anions bearing names ending in -ate or in -ite may also be treated as in **5.1**, but names more in accordance with custom are formed by using the terminations -ic acid and -ous acid corresponding with the anion terminations -ate and -ite, respectively. Thus chloric acid corresponds to chlorate, sulfuric acid to sulfate, and phosphorous acid to phosphite.

This nomenclature may also be used for less common acids, *e.g.*, hexacyanoferric acids correspond to hexacyanoferrate ions. In such cases, however, systematic names of the type hydrogen hexacyanoferrate are preferable.

Most of the common acids are oxo acids, *i.e.*, they contain only oxygen atoms bound to the characteristic atom. It is a long-established custom not to indicate these oxygen atoms. It is mainly for these acids that long-established names will have to be retained. Most other acids may be considered as coördination compounds and be named as such.

◆ Polyatomic means heteratomic here, as opposed to pseudobinary. *Cf.* comment at 3.12.

5.21. Oxo Acids.—For the oxo acids the ous–ic notation to distinguish between different oxidation states is applied in many cases. The -ous acid names are restricted to acids corresponding to the -ite anions listed in the table in **3.224**.

Further distinction between different acids with the same characteristic element is in some cases effected by means of prefixes. This notation should not be extended beyond the cases listed below.

5.211.—The prefix hypo- is used to denote a lower oxidation state, and may be retained in these cases

$H_4B_2O_4$	hypoboric acid
$H_2N_2O_2$	hyponitrous acid
$H_4P_2O_6$	hypophosphoric acid
HPH_2O_2	hypophosphorous acid
HOCl	hypochlorous acid (and similarly for the other halogens)

5.212.—The prefix per- is used to designate a higher oxidation state and may be retained for

$HClO_4$, perchloric acid, and similarly for the other elements in Group VII.

The prefix per- should not be confused with the prefix peroxo- (see **5.22**).

5.213.—The prefixes ortho- and meta- have been used to distinguish acids differing in "water content." These names are approved

H_3BO_3	orthoboric acid
H_4SiO_4	orthosilicic acid
H_3PO_4	orthophosphoric acid
H_5IO_6	orthoperiodic acid
H_6TeO_6	orthotelluric acid
$(HBO_2)_n$	metaboric acids
$(H_2SiO_3)_n$	metasilicic acids
$(HPO_3)_n$	metaphosphoric acids

For the acids derived by removing water from orthoperiodic or orthotelluric acid, the systematic names should be used, *e.g.*, HIO_4 tetraoxoiodic(VII) acid.

The prefix pyro- has been used to designate an acid formed from two molecules of an ortho acid minus one molecule of water. Such acids can now generally be regarded as the simplest cases of isopoly acids (*cf.* **7.5**). The prefix pyro- may be retained for pyrosulfurous and pyrosulfuric acids and for pyrophosphorous and pyrophosphoric acids, although in these cases also the prefix di- is preferable.

◆ The use of orthoperiodic acid and orthotelluric acid is approved, but the question of names for HIO_4, *etc.*, needs further study because of confusion in the literature.

5.214.—The accompanying Table II contains the accepted names of the oxo acids (whether known in the free state or not) and some of their thio and peroxo derivatives (**5.22** and **5.23**).

For the less common of these acids systematic names would seem preferable, for example

H_2MnO_4	manganic(VI) acid, to distinguish it from H_3MnO_4, manganic(V) acid
$HReO_4$	tetraoxorhenic(VII) acid, to distinguish it from H_3ReO_5, pentaoxorhenic(VII) acid
H_2ReO_4	tetraoxorhenic(VI) acid, to distinguish it from $HReO_3$, trioxorhenic(V) acid; H_3ReO_4, tetraoxorhenic(V) acid; and $H_4Re_2O_7$, heptaoxodirhenic(V) acid
H_2NO_2	dioxonitric(II) acid instead of nitroxylic acid.

Trivial names should not be given to such acids as HNO, $H_2N_2O_3$, $H_2N_2O_4$, of which salts have been described. These salts are to be designated systematically as oxonitrates(I), trioxodinitrates(II), tetraoxodinitrates(III), respectively.

The names germanic acid, stannic acid, antimonic acid, bismuthic acid, vanadic acid, niobic acid, tantalic acid, telluric acid, molybdic acid, wolframic acid, and uranic acid may be used for substances with indefinite "water content" and degree of polymerization.

◆ Unless trivial names clash with good nomenclature practices or are ambiguous, retention of well-established ones or the use of formulas is urged (especially for HNO, $H_2N_2O_3$, *etc.*) until structures are known. Systematic coördination-type names in the case of these nitrogen acids, for example, imply a structure that is ruled out by our present state of knowledge.

If hexahydroxoantimonic acid is considered a trivial name, hexahydroxy- might be preferable (*cf.* the systematic name hexahydroxoantimonate(V) ion in 3.223). For the analogous use of peroxo and peroxy, see comment at 5.22.

TABLE II

NAMES FOR OXO ACIDS

H_3BO_3	orthoboric acid or (mono)boric acid
$(HBO_2)_n$	metaboric acids
$(HBO_2)_3$	trimetaboric acid
$H_4B_2O_4$	hypoboric acid
H_2CO_3	carbonic acid
HOCN	cyanic acid
HNCO	isocyanic acid
HONC	fulminic acid
H_4SiO_4	orthosilicic acid
$(H_2SiO_3)_n$	metasilicic acids
HNO_3	nitric acid
HNO_4	peroxonitric acid
HNO_2	nitrous acid
HOONO	peroxonitrous acid
H_2NO_2	nitroxylic acid
$H_2N_2O_2$	hyponitrous acid
H_3PO_4	(ortho)phosphoric acid
$H_4P_2O_7$	diphosphoric or pyrophosphoric acid
$H_5P_3O_{10}$	triphosphoric acid
$H_{n+2}P_nO_{3n+1}$	polyphosphoric acids
$(HPO_3)_n$	metaphosphoric acids
$(HPO_3)_3$	trimetaphosphoric acid
$(HPO_3)_4$	tetrametaphosphoric acid
H_3PO_5	peroxo(mono)phosphoric acid
$H_4P_2O_8$	peroxodiphosphoric acid
$(HO)_2OP\text{–}PO(OH)_2$	hypophosphoric acid
$(HO)_2P\text{–}O\text{–}PO(OH)_2$	diphosphoric(III,V) acid
H_2PHO_3	phosphorous acid
$H_4P_2O_5$	diphosphorous or pyrophosphorous acid
HPH_2O_2	hypophosphorous acid
H_3AsO_4	arsenic acid
H_3AsO_3	arsenious acid
$HSb(OH)_6$	hexahydroxoantimonic acid
H_2SO_4	sulfuric acid
$H_2S_2O_7$	disulfuric or pyrosulfuric acid
H_2SO_5	peroxo(mono)sulfuric acid
$H_2S_2O_8$	peroxodisulfuric acid
$H_2S_2O_3$	thiosulfuric acid
$H_2S_2O_6$	dithionic acid
H_2SO_3	sulfurous acid
$H_2S_2O_5$	disulfurous or pyrosulfurous acid
$H_2S_2O_2$	thiosulfurous acid
$H_2S_2O_4$	dithionous acid
H_2SO_2	sulfoxylic acid
$H_2S_xO_6$ $(x = 3,4\ldots)$	polythionic acids
H_2SeO_4	selenic acid
H_2SeO_3	selenious acid
H_6TeO_6	(ortho)telluric acid
H_2CrO_4	chromic acid
$H_2Cr_2O_7$	dichromic acid
$HClO_4$	perchloric acid
$HClO_3$	chloric acid
$HClO_2$	chlorous acid
HClO	hypochlorous acid
$HBrO_3$	bromic acid
$HBrO_2$	bromous acid
HBrO	hypobromous acid
H_5IO_6	(ortho)periodic acid
HIO_3	iodic acid
HIO	hypoiodous acid
$HMnO_4$	permanganic acid
H_2MnO_4	manganic acid
$HTcO_4$	pertechnetic acid
H_2TcO_4	technetic acid
$HReO_4$	perrhenic acid
H_2ReO_4	rhenic acid

5.22. Peroxo Acids.—The prefix peroxo, when used in conjunction with the trivial names of acids, indicates substitution of –O– by –O–O– (*cf.* **7.312**).

Examples:

HNO_4	peroxonitric acid
H_3PO_5	peroxophosphoric acid
$H_4P_2O_8$	peroxodiphosphoric acid
H_2SO_5	peroxosulfuric acid
$H_2S_2O_8$	peroxodisulfuric acid

◆ Peroxy, as recommended in the 1940 Rules (inorganic), is more acceptable than peroxo to organic chemists. It is not necessary that the use with trivial names conform with the use of peroxo denoting a coördinated ligand; *e.g.*, peroxysulfuric acid or trioxoperoxosulfuric(VI) acid.

5.23. Thio Acids.—Acids derived from oxo acids by replacement of oxygen by sulfur are called *thio acids* (*cf.* **7.312**).

Examples:

$H_2S_2O_2$	thiosulfurous acid
$H_2S_2O_3$	thiosulfuric acid
HSCN	thiocyanic acid

When more than one oxygen atom can be replaced by sulfur the number of sulfur atoms generally should be indicated

H_3PO_3S	monothiophosphoric acid
$H_3PO_2S_2$	dithiophosphoric acid
H_2CS_3	trithiocarbonic acid
H_3AsS_3	trithioarsenious acid
H_3AsS_4	tetrathioarsenic acid

The prefixes seleno- and telluro- may be used in a similar manner.

5.24. Chloro Acids, etc.—Acids containing ligands other than oxygen and sulfur are generally designated according to the rules in Section **7**.

Examples:

$HAuCl_4$	hydrogen tetrachloroaurate(III) or tetrachloroauric(III) acid
H_2PtCl_4	hydrogen tetrachloroplatinate(II) or tetrachloroplatinic(II) acid
H_2PtCl_6	hydrogen hexachloroplatinate(IV) or hexachloroplatinic(IV) acid
$H_4Fe(CN)_6$	hydrogen hexacyanoferrate(II) or hexacyanoferric(II) acid
$H[PHO_2F]$	hydrogen hydridodioxofluorophosphate or hydridodioxofluorophosphoric acid
HPF_6	hydrogen hexafluorophosphate or hexafluorophosphoric acid
H_2SiF_6	hydrogen hexafluorosilicate or hexafluorosilicic acid
H_2SnCl_6	hydrogen hexachlorostannate(IV) or hexachlorostannic(IV) acid
HBF_4	hydrogen tetrafluoroborate or tetrafluoroboric acid
$H[B(OH)_2F_2]$	hydrogen dihydroxodifluoroborate or dihydroxodifluoroboric acid
$H[B(C_6H_5)_4]$	hydrogen tetraphenylborate or tetraphenylboric acid

It is preferable to use names of the type hydrogen tetrachloroaurate(III).

For some of the more important acids of this type abbreviated names may be used, *e.g.*, chloroplatinic acid, fluorosilicic acid.

◆ For the use of hydrido in the fifth example see comment at 7.312.

5.3. Functional Derivatives of Acids

Functional derivatives of acids are compounds formed from acids by substitution of OH and sometimes also O by other groups. In this borderline between organic and inorganic chemistry organic-chemical nomenclature principles prevail.

◆ The intention of the statement "organic-chemical nomenclature principles prevail" is not clear, since most of the examples given in the sections immediately following are not named according to organic practice. *Cf.* 3.33.

5.31. Acid Halides.—The names of acid halides are formed from the name of the corresponding acid radical if this has a special name, *e.g.*, sulfuryl chloride, phosphoryl chloride.

In other cases these compounds are named as oxide halides according to rule **6.41**, *e.g.*, MoO_2Cl_2, molybdenum dioxide dichloride.

5.32. Acid Anhydrides.—Anhydrides of inorganic acids generally should be given names as oxides, *e.g.*, N_2O_5 dinitrogen pentaoxide, ***not*** nitric anhydride or nitric acid anhydride.

5.33. Esters.—Esters of inorganic acids are given names in the same way as the salts, *e.g.*, dimethyl sulfate, diethyl hydrogen phosphate.

If, however, it is desired to specify the constitution of the compound, a name based on the nomenclature for coördination compounds should be used.

Example:

$(CH_3)_4[Fe(CN)_6]$	tetramethyl hexacyanoferrate(II)
or	or
$[Fe(CN)_2(CH_3NC)_4]$	dicyanotetrakis(methyl isocyanide)iron(II)

◆ According to common organic practice for esters (ethers, sulfides, *etc.*) and to the naming of inorganic salts (*e.g.*, sodium sulfate, not disodium sulfate), methyl sulfate would be used instead of dimethyl sulfate. However, no objection is seen to the more specific name. Such names as methyl sulfate are better for alphabetic listing, as in indexes.

5.34. Amides.—The names for amides may be derived from the names of acids by replacing acid by amide, or from the names of the acid radicals.

Examples:

$SO_2(NH_2)_2$	sulfuric diamide or sulfonyl diamide
$PO(NH_2)_3$	phosphoric triamide or phosphoryl triamide

If not all hydroxyl groups of the acid have been replaced by NH_2 groups, names ending in -amidic acid may be used: this is an alternative to naming the compounds as complexes.

Examples:

NH_2SO_3H	amidosulfuric acid or sulfamidic acid
$NH_2PO(OH)_2$	amidophosphoric acid or phosphoramidic acid
$(NH_2)_2PO(OH)$	diamidophosphoric acid or phosphorodiamidic acid

Abbreviated names (sulfamide, phosphamide, sulfamic acid) are often used but are not recommended.

◆ The use of adjectives from names of inorganic acids may lead to confusion because an -ic or -ous adjective (as chromic) may refer to a higher- or lower-valent form of the element as well as to the acid (a possibility that does not arise, of course, with adjectives from names of organic acids).

Names of the type phosphoramidic acid are recommended in the report of the Advisory Committee on the Nomenclature of Organic Phosphorus Compounds of the Division of Organic Chemistry of the ACS published in 1952, but are not as acceptable to the inorganic nomenclature committees as a whole as the amido- or coördination-type names. *Cf.* 3.33.

The retention of sulfamic acid and sulfamide as trivial names is favored by the committees. An acceptable systematic name for NH_2SO_3H would be ammonia–sulfur trioxide, in keeping with its probable structure.

5.35. Nitriles.—The suffix -nitrile has been used in the names of a few inorganic compounds, *e.g.*, $(PNCl_2)_3$, trimeric phosphonitrile chloride. According to **2.22** such compounds can be designated as nitrides, *e.g.*, phosphorus nitride dichloride. Accordingly there seems to be no reason for retention of the name nitrile (and nitrilo, *cf.* **3.33**) in inorganic chemistry.

◆ Nitrilo is used in organic chemistry, though not given in the list at the end of the Rules.

6. SALTS AND SALT-LIKE COMPOUNDS

Among salts particularly there persist many old names which are bad and misleading, and the Commission wishes to emphasize that any which do not conform to these Rules should be discarded.

6.1. Simple Salts

Simple salts fall under the broad definition of binary compounds given in Section 2, and their names are formed from those of the constituent ions (given in Section 3) in the manner set out in Section 2.

6.2. Salts Containing Acid Hydrogen ("Acid" Salts[1])

Names are formed by adding the word hydrogen, to denote the replaceable hydrogen present, immediately in front of the name of the anion.

The nonacidic hydrogen present, *e.g.*, in the phosphite ion, is included in the name of the anion and is not explicitly cited (*e.g.*, Na_2PHO_3, sodium phosphite).

Examples:

$NaHCO_3$	sodium hydrogen carbonate
NaH_2PO_4	sodium dihydrogen phosphate
$NaH[PHO_3]$	sodium hydrogen phosphite

◆ The use of "fused" hydrogen names (as hydrogencarbonate in the original version) is not acceptable in English; the present practice of running hydrogen as a separate word is preferred and has been followed throughout this version. *Cf.* 3.222, 6.324, 6.333. If necessary for clarity, parentheses can be used, as in naming ligands, *e.g.*, (hydrogen carbonato). The use of hydro (as in hydrocarbonato) is not acceptable because of conflicts with organic usage, where hydro denotes addition of hydrogen to unsaturated compounds.

It seems safer to cite even nonacidic hydrogen present in an anion like PHO_3^{2-} (unless the ion has a specific name), because of current usage. (*Cf.* triethyl phosphite in 7.412, seventh example).

6.3. Double Salts, Triple Salts, etc.

6.31.—In formulas all the cations shall precede the anions; in names the principles embodied in Section 2 shall be applied. In those languages where cation names are placed after anion names the adjectives double, triple, *etc.* (their equivalents in the language concerned) may be added immediately after the anion name. The number so implied concerns the number of *kinds* of cation present and *not* the total number of such ions.

6.32.—Cations.

6.321.—Cations shall be arranged in order of increasing valence (except hydrogen, *cf.* **6.2** and **6.324**).

6.322.—The cations of each valence group shall be arranged in order of decreasing atomic number, with the polyatomic radical ions (*e.g.*, ammonium) at the end of their appropriate group.

◆ Alphabetical order would be simpler here and even for 6.321.

6.323. Hydration of Cations.—Owing to the prevalence of hydrated cations, many of which are in reality complex, it seems unnecessary to disturb the cation order in order to allow for this; but if it is necessary to draw attention specifically to the presence of a particular hydrated cation this may be done by writing, for example, "hexaaquo" or "tetraaquo" before the name of the simple ion. Apart from this exception, however, all complex ions should be placed after the simple ones in the appropriate valence group.

◆ *Cf.* comment at 7.322.

6.324. Acidic Hydrogen.—When hydrogen is considered to be present as a cation its name shall be cited last among the cations. Actually acidic hydrogen will in most cases be bound to an anion and shall be cited together with this (**6.2**). If the salt contains only one anion, acidic hydrogen shall be cited in the same place whichever view is taken of the function of this hydrogen. Nonacidic hydrogen shall be either not explicitly cited (*cf.* **6.2**) or designated hydrido (*cf.* **5.24** and **7.311**). For salts with more than one anion see **6.333**.

Examples:

$KMgF_3$
potassium magnesium fluoride

$TlNa(NO_3)_2$
thallium(I) sodium nitrate or thallium sodium dinitrate

$KNaCO_3$
potassium sodium carbonate

$NH_4MgPO_4.6H_2O$
ammonium magnesium phosphate hexahydrate

$NaZn(UO_2)_3(C_2H_3O_2)_9.6H_2O$
sodium zinc triuranyl acetate hexahydrate

$Na[Zn(H_2O)_6](UO_2)_3(C_2H_3O_2)_9$
sodium hexaaquozinc triuranyl acetate

$NaNH_4HPO_4.4H_2O$
sodium ammonium hydrogen phosphate tetrahydrate

◆ *Cf.* comments at 6.2, 7.312. In the fifth and sixth examples, either triuranyl(VI) or nonaacetate should be specified. *Cf.* 3.32, 6.34.

6.33.—Anions.

6.331.—Anions are to be cited in this group order

1. H^-
2. O^{2-} and OH^- (in that order)
3. Simple (*i.e.*, one element only) inorganic anions, other than H^- and O^{2-}
4. Inorganic anions containing two or more elements, other than OH^-
5. Anions of organic acids and organic substances exerting an acid function

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[1] For "basic" salts see 6.4.

◆ The committees consider it preferable to cite H^- last in accordance with usage.

6.332.—Within group 3 the ions shall be cited in the order given in 2.16, the inclusion of O in that list being taken as referring to all oxygen anions apart from O^{2-} (*i.e.*, $O_2{}^{2-}$, *etc.*).

Within group 4, anions containing the smallest number of atoms shall be cited first, and in the case of two ions containing the same number of atoms they shall be cited in order of decreasing atomic number of the central atoms. Thus $CO_3{}^{2-}$ should precede $CrO_4{}^{2-}$, and the latter should precede $SO_4{}^{2-}$.

Within group 5 the anions shall be cited in alphabetical order.

◆ Again alphabetical order would be simpler, within groups 3 and 4 as well as 5. *Cf.* comment at 7.251.

6.333.—Acidic hydrogen should be cited together with the anion to which it is attached. If it is not known to which anion the hydrogen is bound, it should be cited last among the cations.

◆ *Cf.* comment at 6.2.

6.34.—The stoichiometric method is the most practicable for indicating the proportions of the constituents. It is not always essential to give the numbers of all the anions, provided the valences of all the cations are either known or indicated.

Examples:

$NaCl.NaF.2Na_2SO_4$ or $Na_6ClF(SO_4)_2$	(hexa)sodium chloride fluoride (bis)sulfate
$Ca_5F(PO_4)_3$	(penta)calcium fluoride (tris)phosphate

The parentheses in these cases mean that numerical prefixes may not be necessary. The multiplicative numerical prefixes bis, tris, *etc.*, should be used in connection with anions, because disulfate, triphosphate, *etc.*, designate isopoly anions.

6.4. Oxide and Hydroxide Salts

("Basic" salts, formerly oxy and hydroxy salts)

6.41.—For the purposes of nomenclature, these should be regarded as double salts containing O^{2-} and OH^- anions, and Section 6.3 may be applied in its entirety.

6.42. Use of the Prefixes Oxy and Hydroxy.—In some languages the citation in full of all the separate anion names presents no trouble and is strongly recommended (*e.g.*, copper oxide chloride), to the exclusion of the oxy form wherever possible. In some other languages, however, such names as "oxyde et chlorure double de cuivre" are so far removed from current practice that the present system of using oxy- and hydroxy-, *e.g.*, oxychlorure de cuivre, may be retained in such cases.

Examples:

$Mg(OH)Cl$	magnesium hydroxide chloride
$BiOCl$	bismuth oxide chloride
$LaOF$	lanthanum oxide fluoride
$VOSO_4$	vanadium(IV) oxide sulfate
$CuCl_2.3Cu(OH)_2$ or $Cu_2(OH)_3Cl$	dicopper trihydroxide chloride
$ZrOCl_2.8H_2O$	zirconium oxide (di)chloride octahydrate

6.5. Double Oxides and Hydroxides

The terms "mixed oxides" and "mixed hydroxides" are not recommended. Such substances preferably should be named double, triple, *etc.*, oxides or hydroxides as the case may be.

Many double oxides and hydroxides belong to several distinct groups, each having its own characteristic structure type, which is sometimes named after some well-known mineral of the same group (*e.g.*, perovskite, ilmenite, spinel). Thus, $NaNbO_3$, $CaTiO_3$, $CaCrO_3$, $CuSnO_3$, $YAlO_3$, $LaAlO_3$, and $LaGaO_3$ all have the same structure as perovskite, $CaTiO_3$. Names such as calcium titanate may convey false implications and it is preferable to name such compounds as double oxides and double hydroxides unless there is clear and generally accepted evidence of cations and oxo or hydroxo anions in the structure. This does not mean that names such as titanates or aluminates should always be abandoned, because such substances may exist in solution and in the solid state (*cf.* 3.223).

◆ "Multiple" has been used in English as a class term including double, triple, etc. (oxides or the like).

6.51.—In the double oxides and hydroxides the metals shall be named in the same order as for double salts (6.32).

6.52.—When required the structure type may be added in parentheses and in italics after the name, except that when the type name is also the mineral name of the substance itself then the italics should not be used (*cf.* 4.2).

Examples:

$NaNbO_3$	sodium niobium trioxide (*perovskite* type)
$MgTiO_3$	magnesium titanium trioxide (*ilmenite* type)
$FeTiO_3$	iron(II) titanium trioxide (ilmenite)
$4CaO.Al_2O_3.nH_2O$ or $Ca_2Al(OH)_7.nH_2O$	dicalcium aluminum hydroxide hydrate
but $Ca_3[Al(OH)_6]_2$	(tri)calcium (bis)-[hexahydroxoaluminate]
$LiAl(OH)_4.2MnO_2$ or $LiAlMn^{IV}{}_2O_4(OH)_4$	lithium aluminum dimanganese(IV) tetraoxide tetrahydroxide

7. COÖRDINATION COMPOUNDS

7.1. Definitions

In its oldest sense the term *coördination compound* is taken as referring to molecules or ions in which there is an atom (A) to which are attached other atoms (B) or groups (C) to a number in excess of that corresponding to the oxidation number of the atom A. However, the system of nomenclature originally evolved for the compounds within this narrow definition has proved useful for a much wider class of compounds, and for the purposes of nomenclature the restriction "in excess . . . oxidation number" is to be omitted. Any compound formed by addition of one or several ions and/or molecules to one or more ions or/and molecules may be named according to the same system as strict coördination compounds.

The effect of this is to bring many simple and well-known compounds under the same nomenclature rules as accepted coördination compounds; the result is to reduce the diversity of names and avoid many controversial issues, because it should be understood that there is no intention of implying that any structural analogy necessarily exists between different compounds merely on account of a common system of nomenclature. The system extends also to many addition compounds.

In the rules which follow certain terms are used in the senses here indicated: the atom referred to above as (A) is known as the *central* or *nuclear* atom, and all other atoms which are directly attached to A are known as *coördinating atoms*. Atoms (B) and groups (C) are called *ligands*. A group containing more than one *potential* coördinating atom is termed a *multidentate* ligand, the number of potential coördinating atoms being indicated by the terms *unidentate, bidentate, etc.* A *chelate* ligand is a ligand *attached* to *one* central atom through *two or more* coördinating atoms, while a *bridging group* is attached to *more than one* atom. The whole assembly of one or more central atoms with their attached ligands is referred to as a *complex*, which may be an uncharged molecule or an ion of either polarity. A *polynuclear complex* is a complex which contains *more than one* nuclear atom, their number being designated by the terms *mononuclear, dinuclear, etc.*

◆ Some dissatisfaction with the definition of coördination compounds was expressed, though the broad definition (last sentence of first paragraph) was generally approved.

Central atom or *center of coördination* is to be preferred to *nuclear* atom because of other senses of nucleus, especially of an atom. Possible replacements for polynuclear, etc., are polycentric, *etc.*, or bridged complex since bridging group is in common use.

In the United States the Greek-Latin hybrid terms polydentate and monodentate seem to be used more than the all-Latin multidentate and unidentate.

7.2. Formulas and Names for Complex Compounds in General

7.21. Central Atoms.—In *formulas* the symbol for the central atom(s) should be placed *first* (except in formulas which are primarily structural), the anionic and neutral, *etc.*, ligands following as prescribed in **7.25**, and the formula for the whole complex entity (ion or molecule) should be placed in brackets [ ].

In *names* the central atom(s) should be placed *after* the ligands.

◆ It is considered preferable to place the whole complex in brackets, especially when more than one central atom is present, but not essential with only one central atom or with complex ions or nonionic complexes, because brackets may be needed sometimes for indicating concentrations.

7.22. Indication of Valence and Proportion of Constituents.—The oxidation number of the central atom is indicated by means of the Stock notation (**2.252**). Alternatively the proportion of constituents may be given by means of stoichiometric prefixes (**2.251**).

7.23.—Formulas and names may be supplemented with the prefixes *cis, trans, etc.* (**2.19**).

7.24. Terminations.—Complex anions shall be given the termination -ate (*cf.* **2.23, 2.24** and **3.223**). Complex cations and neutral molecules are given no distinguishing termination. For further details concerning the names of ligands see **7.3**.

7.25. Order of Citation of Ligands in Complexes.—

first: anionic ligands
next: neutral and cationic ligands

7.251.—The anionic ligands shall be cited in the order

1. H^-
2. O^{2-}, OH^- (in that sequence)
3. Other simple anions (*i.e.*, one element only)
4. Polyatomic anions
5. Organic anions in alphabetical order

The sequence within categories 3 and 4 should be that given in **6.332**.

◆ H^- is preferably named last, not first (*cf.* comment at 6.331). Alphabetical order is strongly recommended for simplicity at least within 3 and 4, where only rare uses are involved. The intention seems to be to include under 3 monatomic ions (*i.e.*, one *atom*—rather than one *element*—only), in other words to exclude N_3, I_3, etc. Under 4 the insertion of "inorganic" between "Polyatomic" and "anions" is recommended.

7.252.—Neutral and cationic ligands shall be cited in the order given

first: water, ammonia (in that sequence)
then: other inorganic ligands in the sequence in which their coördinating elements appear in the list given in **2.16**
last: organic ligands in alphabetical order.

◆ For the inorganic ligands alphabetical order again is recommended. The use of parentheses wherever there is any possibility of ambiguity should be stressed, as illustrated in examples under 7.321: potassium trichloro(ethylene)-platinate(II), where parentheses are given in the Rules, and tetra(pyridine)platinum(II) tetrachloroplatinate(II), where they have been added in this version. Parentheses might also be helpful with "thiocyanato" preceded by a numerical prefix (see last example in 7.311) and are definitely required with two-word names for ligands recommended instead of the fused names of the original version (6.2), as in the seventh example in 7.412: di-*μ*-carbonyl-bis{carbonyl(triethyl phosphite)cobalt}. Since brackets denote complexes, braces can be used in formulas or names where needed in order to avoid the use of two sets of parentheses (braces were so used in some but not all such cases in the original version).

7.3. Names for Ligands

7.31.—Anionic Ligands.

7.311.—The names for anionic ligands, whether inorganic or organic, end in -o (see, however, **7.324**). In general, if the anion name ends in -ide, -ite, or -ate, the final -e is replaced by -o, giving -ido, -ito, and -ato, respectively.

Examples:

$Li[AlH_4]$
lithium tetrahydridoaluminate
$Na[BH_4]$
sodium tetrahydridoborate
$K_2[OsNCl_5]$
potassium nitridopentachloroösmate(VI)
$[Co(NH_2)_2(NH_3)_4]OC_2H_5$
diamidotetraamminecobalt(III) ethanolate
$[CoN_3(NH_3)_5]SO_4$
azidopentaamminecobalt(III) sulfate
$Na_3[Ag(S_2O_3)_2]$
sodium bis(thiosulfato)argentate(I)
$[Ru(HSO_3)_2(NH_3)_4]$
bis(hydrogen sulfito)tetraammineruthenium
(II) $NH_4[Cr(SCN)_4(NH_3)_2]$
ammonium tetrathiocyanatodiamminechromate(III)

◆ For "ethanolate" in the fourth example "ethoxide" may be preferred.

7.312.—These anions do not follow exactly the above rule; modified forms have become established:

F^-	fluoride	fluoro (*not* fluo)
Cl^-	chloride	chloro
Br^-	bromide	bromo
I^-	iodide	iodo
O^{2-}	oxide	oxo
OH^-	hydroxide	hydroxo
O_2^{2-}	peroxide	peroxo
HS^-	hydrogen sulfide	thiolo
S^{2-}	sulfide	thio[1] (sulfido)
(but:S_2^{2-}	disulfide	disulfido)
CN^-	cyanide	cyano

By analogy with hydroxo, CH_3O^-, *etc.*, are called methoxo, *etc.* For CH_3S^-, *etc.*, the systematic names methanethiolato, *etc.*, are used.

Examples:

$K[AgF_4]$
potassium tetrafluoroargentate(III)

$K_2[NiF_6]$
potassium hexafluoroniccolate(IV)

$Ba[BrF_4]_2$
barium tetrafluorobromate(III)

$Na[AlCl_4]$
sodium tetrachloroaluminate

$Cs[ICl_4]$
cesium tetrachloroiodate(III)

$K[Au(OH)_4]$
potassium tetrahydroxoaurate(III)

$K[CrOF_4]$
potassium oxotetrafluorochromate(V)

$K_2[Cr(O)_2O_2(CN)_2(NH_3)]$
potassium dioxoperoxodicyanoamminechromate(VI)

$Na[BH(OCH_3)_3]$
sodium hydridotrimethoxoborate

$K_2[Fe_2S_2(NO)_4]$
dipotassium dithiotetranitrosyldiferrate

◆ It is strongly recommended on the basis of past and present usage, analogy with chloro, *etc.*, and euphony that hydro be added to the list of modified forms of names for anionic ligands and that hydrido be abandoned (*cf.* also examples in 7.311).

While the Subcommittee on Coördination Compounds recognizes the usefulness of the invariable -o ending for anionic ligands, some members of the general committees do not see a sharp enough distinction between such ligands and the same groups in organic compounds to justify a departure from organic usage by using hydroxo, methoxo, *etc.*, instead of hydroxy, methoxy, *etc.* These members therefore favor adding hydroxy, methoxy, *etc.*, to the hydrocarbon radicals excepted from the rule of -o endings for anions (7.324). For the use of peroxo, see comment at 5.22.

The -o of a negative ligand should not be elided before another vowel (chloroösmate, chloroiodo). This agrees with organic practice. *Cf.* comment at 7.322.

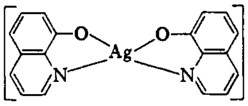
It should be pointed out here as well as in the list of names for ions and radicals at the end of the Rules that the approved organic name for unsubstituted HS is mercapto (not thiol, as also given in the list) and for the alkyl- and aryl-substituted radicals methylthio, *etc.*

7.313.—Ligands derived from organic compounds not normally called acids, but which function as such in complex formation by loss of a proton, should be treated as anionic and given the ending -ato. If, however, no proton is lost, the ligand must be treated as neutral—see **7.32.**

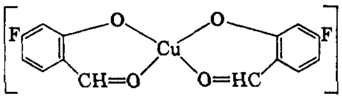
Examples:

$[Ni(C_4H_7N_2O_2)_2]$ bis(dimethylglyoximato) nickel(II)

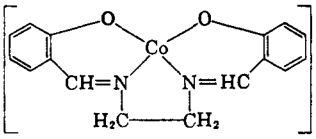
$[Cu(C_5H_7O_2)_2]$ bis(acetylacetonato)copper(II)



bis(8-quinolinolato)-silver(II)



bis(4-fluorosalicylaldehydato)copper(II)



N,N′-ethylenebis-(salicylideneiminato)cobalt(II)

◆ Although according to 3.33 the name for the ligand in the second example should be derived from the systematic name 2,4-pentanedione instead of from acetylacetone, acetylacetonato perhaps conveys better the idea that it is the enol form that is involved. However, the coördination subcommittee questions the use of the termination -ato rather than plain -o especially in cases where the -ate terms (as dimethylglyoximate) are not accepted organic practice. Such -ato terms are especially misleading in the last two examples, where the -ato belongs with the hydroxyl part of the name, not the aldehyde or imine part to which it is attached.

7.32.—Neutral and Cationic Ligands.

7.321.—The name of the coördinated molecule or cation is to be used without change, except in the special cases provided for in **7.322.**

Examples:

$[CoCl_2(C_4H_8N_2O_2)_2]$
dichlorobis(dimethylglyoxime)cobalt(II) (*cf.* nickel derivative given in **7.313**)

cis-$[PtCl_2(Et_3P)_2]$
cis-dichlorobis(triethylphosphine)platinum(II)

$[CuCl_2(CH_3NH_2)_2]$
dichlorobis(methylamine)copper(II)

$[Pt\ py_4][PtCl_4]$
tetra(pyridine)platinum(II) tetrachloroplatinate(II)

$[Fe(dipy)_3]Cl_2$
tris(dipyridyl)iron(II) chloride

$[Co\ en_3]_2(SO_4)_3$
tris(ethylenediamine)cobalt(III) sulfate

$[Zn\{NH_2CH_2CH(NH_2)CH_2NH_2\}_2]I_2$
bis(1,2,3-triaminopropane)zinc iodide

$K[PtCl_3(C_2H_4)]$
potassium trichloro(ethylene)platinate(II) or potassium trichloromonoethyleneplatinate(II)

$[PtCl_2\{H_2NCH_2CH(NH_2)CH_2NH_3\}]Cl$
dichloro(2,3 - diaminopropylammonium)platinum(II) chloride

$[Cr(C_6H_5NC)_6]$
hexakis(phenyl isocyanide)chromium

◆ In the fifth example, bipyridine is preferred to dipyridyl in organic practice, and in the seventh example 1,2,3-propanetriamine to 1,2,3-triaminopropane.

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[1] The name thio has long been used to denote the ligand S^{2-} when it can be regarded as replacing O^{2-} in an oxo acid or its anion. The general use of this name will prevent confusion between the two interpretations of disulfido as S_2^{2-} or two S^{2-} ligands.

7.322.—Water and ammonia as neutral ligands in coördination complexes are called "aquo" and "ammine," respectively.

In the tentative rules it was proposed to change the old-established "aquo" to "aqua," thus keeping the -o termination consistently for anionic ligands alone. However, as the old form is so widely used, many regarded the change as too pedantic, and the Commission has decided to retain "aquo" as an exception.

Examples:

$[Cr(H_2O)_6]Cl_3$
hexaaquochromium(III) chloride or hexaaquochromium trichloride

$[Al(OH)(H_2O)_5]^{++}$
the hydroxopentaaquoaluminum ion

$[Co(NH_3)_6]ClSO_4$
hexaamminecobalt(III) chloride sulfate

$[CoCl(NH_3)_5]Cl_2$
chloropentaamminecobalt(III) chloride

$[CoCl_3(NH_3)_2\{(CH_3)_2NH\}]$
trichlorodiammine(dimethylamine)cobalt(III)

◆ Hexaquo, pentaquo, *etc.*, are used in the examples in the original version, but have been changed in this version to hexaaquo, *etc.*, for conformity with the latest approved organic practice. (*Cf.* hexaammonium, given with two a's separated by a hyphen in 7.6, second example, in the original version.)

7.323.—The groups NO, NS, CO, and CS, when linked directly to a metal atom, are to be called nitrosyl, thionitrosyl, carbonyl, and thiocarbonyl, respectively. In computing the oxidation number these radicals are treated as neutral.

Examples:

$Na_2[Fe(CN)_5NO]$
disodium pentacyanonitrosylferrate

$K_3[Fe(CN)_5CO]$
tripotassium pentacyanocarbonylferrate

$K[Co(CN)(CO)_2(NO)]$
potassium cyanodicarbonylnitrosylcobaltate(0)

$HCo(CO)_4$
hydrogen tetracarbonylcobaltate(−I)

$[Ni(CO)_2(Ph_3P)_2]$
dicarbonylbis(triphenylphosphine)nickel(0)

$[Fe\ en_3][Fe(CO)_4]$
tris(ethylenediamine)iron(II) tetracarbonylferrate (−II)

$Mn_2(CO)_{10}$ or $[(CO)_5Mn-Mn(CO)_5]$
decacarbonyldimanganese(0) or bis(pentacarbonylmanganese)

◆ The necessity of arbitrarily considering these groups as always neutral can be avoided by not using the oxidation number but instead the stoichiometric proportions (as in some of these examples) or the Ewens–Bassett system (*cf.* comment at 2.252). Thus the anion in the last example in 7.312 (where NO is known to be positive) would by this system be named dithiotetranitrosyldiferrate(2−).

7.324.—Anions derived from hydrocarbons are given radical names without -o, but are counted as negative when computing the oxidation number.

The consistent introduction of the ending -o would in this case lead to unfamiliar names, *e.g.*, phenylato or phenido for $C_6H_5^-$. On the other hand, if the radicals were counted as neutral ligands, the central atom would have to be given an unusual oxidation number, *e.g.*, −I for boron in $K[B(C_6H_5)_4]$, instead of III.

Examples:

$K[B(C_6H_5)_4]$
potassium tetraphenylborate

$K[SbCl_5C_6H_5]$
potassium pentachloro(phenyl)antimonate(V)

$K_2[Cu(C_2H)_3]$
potassium triethynylcuprate(I)

$K_4[Ni(C_2C_6H_5)_4]$
potassium tetrakis(phenylethynyl)niccolate(0)

$[Fe(CO)_4(C_2C_6H_5)_2]$
tetracarbonylbis(phenylethynyl)iron(II)

$Fe(C_5H_5)_2$
bis(cyclopentadienyl)iron(II)

$[Fe(C_5H_5)_2]Cl$
bis(cyclopentadienyl)iron(III) chloride

$[Ni(NO)(C_5H_5)]$
nitrosylcyclopentadienylnickel

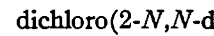
◆ The use of radical names such as cyclopentadienyl in the examples does not seem consistent with the use of Stock notations; for the sixth example ("ferrocene"), iron(II) cyclopentadienide is preferred by some. This matter is presumably part of the whole organometallic problem to be dealt with by the new IUPAC joint organic-inorganic subcommittee.

For niccolate, see comment at 1.12.

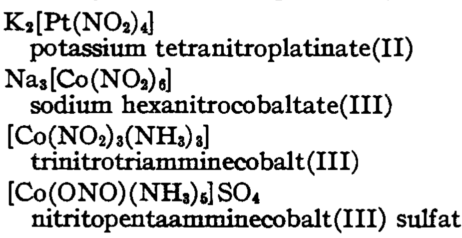
7.33.—Alternative Modes of Linkage of Some Ligands.—Where ligands are capable of attachment by different atoms this may be denoted by adding the symbol for the atom by which attachment occurs at the end of the name of the ligand. Thus the dithioöxalato group may be attached through S or O, and these are distinguished as dithioöxalato-*S*,*S′* and dithioöxalato-*O*,*O′*, respectively.

In some cases different names are already in use for alternative modes of attachment, as, for example, thiocyanato (−SCN) and isothiocyanato (−NCS), nitro ($-NO_2$), and nitrito (−ONO). In these cases existing custom may conveniently be retained.

Examples:



potassium bis(dithioöxalato-*S*,*S′*)niccolate(II)



dichloro(2-*N*,*N*-dimethylaminoethyl 2-aminoethyl sulfide-*N′*,*S*)platinum(II)

$K_2[Pt(NO_2)_4]$
potassium tetranitroplatinate(II)

$Na_3[Co(NO_2)_6]$
sodium hexanitrocobaltate(III)

$[Co(NO_2)_3(NH_3)_3]$
trinitrotriamminecobalt(III)

$[Co(ONO)(NH_3)_5]SO_4$
nitritopentaamminecobalt(III) sulfate

$[Co[NCS)(NH_3)_5]Cl_2$
isothiocyanatopentaamminecobalt(III) chloride

◆ Thioöxalato in the original version has been changed to dithioöxalato.

7.4. Di- and Polynuclear Compounds

7.41.—Bridging Groups.

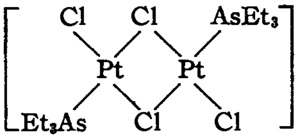
7.411.—A bridging group shall be indicated by adding the Greek letter μ immediately before its name and separating this from the rest of the complex by a hyphen. Two or more bridging groups of the same kind are indicated by di-μ-, *etc.*

7.412.—If the number of central atoms bound by one bridging group exceeds two, the number shall be indicated by adding a subscript numeral to the μ.

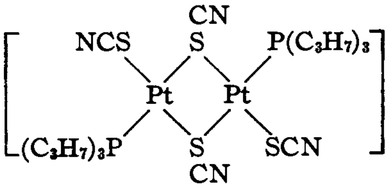
This system of notation allows simply of distinction between, for example, μ-disulfido (one S_2 bridge) and di-μ-sulfido (two S bridges). It is also capable of extension to much more complex and unsymmetrical structures by use of the conventional prefixes *cis*, *trans*, *asym*, and *sym* where necessary.

Examples:

$[(NH_3)_5Cr\text{-}OH\text{-}Cr(NH_3)_5]Cl_5$
μ-hydroxo-bis{pentaamminechromium(III)} chloride



di-μ-chloro-dichlorobis(triethylarsine)diplatinum(II) (three possible isomers: *asym*, *sym-cis*, and *sym-trans;* the last is shown)



di-μ-thiocyanato-dithiocyanatobis(tripropylphosphine)diplatinum(II)

$[(CO)_3Fe(CO)_3Fe(CO)_3]$
tri-μ-carbonyl-bis(tricarbonyliron)

$[(CO)_3Fe(SEt)_2Fe(CO)_3]$
di-μ-ethanethiolato-bis(tricarbonyliron)

$[(C_5H_5)(CO)Fe(CO)_2Fe(CO)(C_5H_5)]$
di-μ-carbonyl-bis(carbonylcyclopentadienyliron)

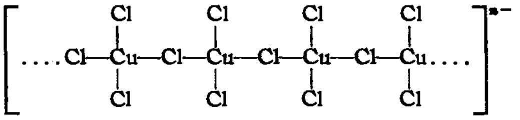
$[(CO)\{P(OEt)_3\}Co(CO)_2Co(CO)\{P(OEt)_3\}]$
di-μ-carbonyl-bis{carbonyl(triethyl phosphite)cobalt}

$[Au(CN)(C_3H_7)_2]_4$
cyclo-tetra-μ-cyano-tetrakis(dipropylgold)

$[CuI(Et_3As)]_4$
tetra-μ_3-iodo-tetrakis{triethylarsinecopper(I)}

$[Be_4O(CH_3COO)_6]$
μ_4-oxo-hexa-μ-acetato-tetraberyllium

7.42. Extended Structures.—Where bridging causes an indefinite extension of the structure it is best to name compounds primarily on the basis of their over-all composition; thus the compound having the composition represented by the formula $CsCuCl_3$ has an anion with the structure:



This may be expressed in the formula $(Cs^+)_n$-$[(CuCl_3)_n]^{n-}$ which leads to the simple name cesium catena-μ-chloro-dichlorocuprate(II). If the structure were in doubt, however, the substance would be called cesium copper(II) chloride (as a double salt).

◆ *Cf.* comment on *catena* at 1.4.

7.5. Isopoly Anions

The structure of many complicated isopoly anions has now been cleared up by X-ray work and it turns out that the indication of the several μ-oxo and oxo atoms in the name does not convey any clear picture of the structure and is therefore of little value.

For the time being it is sufficient to indicate the number of atoms by Greek prefixes, at least until isomers are found. When all atoms have their "normal" oxidation states (*e.g.*, W^{VI}), it is not necessary to give the numbers of the oxygen atoms, if all the others are indicated.

Examples:

$K_2S_2O_7$	dipotassium disulfate
$K_2S_3O_{10}$	dipotassium trisulfate
$Na_5P_3O_{10}$	pentasodium triphosphate
$K_2Cr_4O_{13}$	dipotassium tetrachromate
$Na_2B_4O_7$	disodium tetraborate
NaB_5O_8	sodium pentaborate
$Ca_3Mo_7O_{24}$	tricalcium heptamolybdate
$Na_7HNb_6O_{19}.15H_2O$	heptasodium monohydrogen hexaniobate-15-water
$K_2Mg_2V_{10}O_{28}.16H_2O$	dipotassium dimagnesium decavanadate-16-water

7.6. Heteropoly Anions

The central atom or atoms should be cited last in the name and first in the formula of the anion (*cf.* 7.21), *e.g.*, wolframophosphate, *not* phosphowolframate.

If the oxidation number has to be given, it may be necessary to place it immediately after the atom referred to and not after the ending -ate, in order to avoid ambiguity.

The method formerly recommended for naming iso- and heteropoly anions by giving the number of atoms in parentheses is not practicable in more complicated cases.

Examples:

$(NH_4)_3PW_{12}O_{40}$
triammonium dodecawolframophosphate

$(NH_4)_6TeMo_6O_{24}.7H_2O$
hexaammonium hexamolybdotellurate heptahydrate

$Li_3HSiW_{12}O_{40}.24H_2O$
trilithium (mono)hydrogen dodecawolframosilicate-24-water

$K_6Mn^{IV}Mo_9O_{32}$
hexapotassium enneamolybdomanganate(IV)

$Na_6P^{V}_{2}Mo_{18}O_{62}$
hexasodium 18-molybdodiphosphate(V)

$Na_4P^{III}_{2}Mo_{12}O_{41}$
tetrasodium dodecamolybdodiphosphate(III)

$K_7Co^{II}Co^{III}W_{12}O_{42}.16H_2O$
heptapotassium dodecawolframocobalt(II)-cobalt(III)ate-16-water

$K_3PV_2Mo_{10}O_{39}$
tripotassium decamolybdodivanadophosphate

◆ The coördination subcommittee would prefer not to have sections 7.5 and 7.6 included under 7 and recommends that they should be studied by a special subcommittee. Some cyclic isomers are already known, and isopoly cations also are being investigated.

Cf. comment at 1.12 for stand on wolframate and wolframo, and 2.251 for nona instead of ennea (fourth example).

Isopoly and heteropoly are not separate words in the original version.

7.7. Addition Compounds

The ending -ate is now the accepted ending for *anions* and should generally not be used for addition compounds. Alcoholates are the *salts* of alcohols and this name should not be used to indicate alcohol of crystallization. Analogously addition compounds containing ether, ammonia, *etc.*, should *not* be termed etherates, ammoniates, *etc.*

However, one exception has to be recognized. According to the commonly accepted meaning of the ending -ate, "hydrate" would be, and was formerly regarded as, the name for a *salt* of water, *i.e.*, what is now known as a hydroxide; the name hydrate has now a very firm position as the name of a compound containing water of crystallization and is allowed also in these Rules to designate water bound in an unspecified way; it is considered to be preferable even in this case to avoid the ending -ate by using the name "water" (or its equivalent in other languages) when possible.

The names of addition compounds may be formed by connecting the names of individual compounds by hyphens (short dashes) and indicating the number of molecules by Arabic numerals. When the added molecules are organic, however, it is recommended to use multiplicative numeral prefixes (bis, tris, tetrakis, *etc.*) instead of Arabic figures to avoid confusion with the organic-chemical use of Arabic figures to indicate position of substituents.

Examples:

$CaCl_2.6H_2O$
calcium chloride–6-water (or calcium chloride hexahydrate)

$3CdSO_4.8H_2O$
3-cadmium sulfate–8-water

$Na_2CO_3.10H_2O$
sodium carbonate–10-water (or sodium carbonate decahydrate)

$AlCl_3.4C_2H_5OH$
aluminum chloride–4-ethanol or –tetrakisethanol

$BF_3.(C_2H_5)_2O$
boron trifluoride–diethyl ether

$BF_3.2CH_3OH$
boron trifluoride–bismethanol

$BF_3.H_3PO_4$
boron trifluoride–phosphoric acid

$BiCl_3.3PCl_5$
bismuth trichloride–3-(phosphorus pentachloride)

$TeCl_4.2PCl_5$
tellurium tetrachloride–2-(phosphorus pentachloride)

$(CH_3)_4NAsCl_4.2AsCl_3$
tetramethylammonium tetrachloroarsenate(III)–2-(arsenic trichloride)

$CaCl_2.8NH_3$
calcium chloride–8-ammonia

$8H_2S.46H_2O$
8-(hydrogen sulfide)–46-water

$8Kr.46H_2O$
8-krypton–46-water

$6Br_2.46H_2O$
6-dibromine–46-water

$8CHCl_3.16H_2S.136H_2O$
8-chloroform–16-(hydrogen sulfide)–136-water

These names are not very different from a pure verbal description which may in fact be used, *e.g.*, calcium chloride with 6 water, compound of aluminum chloride with 4 ethanol, *etc.*

If it needs to be shown that added molecules form part of a complex, the names are given according to **7.2** and **7.3.**

Examples:

$FeSO_4.7H_2O$ or $[Fe(H_2O)_6]SO_4.H_2O$
iron(II) sulfate heptahydrate or hexaaquoiron(II) sulfate monohydrate

$PtCl_2.2PCl_3$ or $[PtCl_2(PCl_3)_2]$
platinum(II) chloride–2-(phosphorus trichloride) or dichlorobis(phosphorus trichloride)-platinum(II)

$AlCl_3.NOCl$ or $NO[AlCl_4]$
aluminum chloride–nitrosyl chloride or nitrosyl tetrachloroaluminate

$BF_3.Et_3N$ or $[BF_3(Et_3N)]$
boron trifluoride–triethylamine or trifluoro(triethylamine)boron

◆ Only some so-called "addition compounds" are known to be coördination compounds, and the formulas and names can show such structures. Those that are lattice compounds and those of unknown structure do not really belong in 7.

The committees like hydrate and ammoniate and see no particular advantage in dropping them (*cf.* the use of hydrate terms in examples in 6.324; 6-hydrate, *etc.*, as well as hexahydrate, *etc.*, are considered acceptable).

No reason can be seen for deviating here from usual organic practice by using multiplicative prefixes with simple names: tetraethanol is just as clear as tetrakisethanol, and dimethanol as bismethanol. Parentheses can always be used if there is danger of any ambiguity.

The use of short dashes ("en" dashes) instead of hyphens between the names (as in the examples here, but not in the original version) makes for greater ease in reading.

It is considered preferable by some to place the electron donor first in both the formulas and name: $(C_2H_5)_2O.BF_3$, diethyl ether–boron trifluoride (note that organic usage favors ethyl ether over diethyl ether).

8. POLYMORPHISM

Minerals occurring in nature with similar compositions have different names according to their crystal structures; thus, zinc blende, wurtzite; quartz, tridymite, and cristobalite. Chemists and metallographers have designated polymorphic mod-

LIST OF NAMES FOR IONS AND RADICALS

In inorganic chemistry substitutive names seldom are used, but the organic-chemical names are shown to draw attention to certain differences between organic and inorganic nomenclature.

Atom or group	Name				
	as neutral molecule	as cation or cationic radical[1]	as anion	as ligand	as prefix for substituent in organic compounds
H	monohydrogen	hydrogen	hydride	hydrido	
F	monofluorine		fluoride	fluoro	fluoro
Cl	monochlorine	chlorine	chloride	chloro	chloro
Br	monobromine	bromine	bromide	bromo	bromo
I	monoiodine	iodine	iodide	iodo	iodo
I_3			triiodide		
ClO		chlorosyl	hypochlorite	hypochlorito	
ClO_2	chlorine dioxide	chloryl	chlorite	chlorito	
ClO_3		perchloryl	chlorate	chlorato	
ClO_4			perchlorate		
IO		iodosyl	hypoiodite		iodoso
IO_2		iodyl			iodyl or iodoxy
O	monoöxygen		oxide	oxo	oxo or keto
O_2	dioxygen		O_2^{2-}: peroxide O_2^{-}: hyperoxide	peroxo	peroxy
HO	hydroxyl		hydroxide	hydroxo	hydroxy
HO_2	(perhydroxyl)		hydrogen peroxide	hydrogen peroxo	hydroperoxy
S	monosulfur		sulfide	thio (sulfido)	thio
HS	(sulfhydryl)		hydrogen sulfide	thiolo	thiol or mercapto
S_2	disulfur		disulfide	disulfido	
SO	sulfur monoxide	sulfinyl (thionyl)			sulfinyl
SO_2	sulfur dioxide	sulfonyl (sulfuryl)	sulfoxylate		sulfonyl
SO_3	sulfur trioxide		sulfite	sulfito	
HSO_3			hydrogen sulfite	hydrogen sulfito	
S_2O_3			thiosulfate	thiosulfato	
SO_4			sulfate	sulfato	
Se	selenium		selenide	seleno	seleno
SeO		seleuinyl			seleninyl
SeO_2		selenonyl			selenonyl
SeO_3	selenium trioxide		selenite	selenito	
SeO_4			selenate	selenato	
Te	tellurium		telluride	telluro	telluro
CrO_2		chromyl			
UO_2		uranyl			
NpO_2		neptunyl			
PuO_2		plutonyl			
AmO_2		americyl			
N	mononitrogen		nitride	nitrido	
N_3			azide	azido	
NH			imide	imido	imino
NH_2			amide	amido	amino
NHOH			hydroxylamide	hydroxylamido	hydroxylamino
N_2H_3			hydrazide	hydrazido	hydrazino
NO	nitrogen oxide	nitrosyl		nitrosyl	nitroso
NO_2	nitrogen dioxide	nitryl		nitro	nitro
ONO			nitrite	nitrito	
NS		thionitrosyl			
$(NS)_n$		thiazyl (*e.g.*, trithiazyl)			
NO_3			nitrate	nitrato	
N_2O_2			hyponitrite	hyponitrito	
P	phosphorus		phosphide	phosphido	
PO		phosphoryl			phosphoroso
PS		thiophosphoryl			
PH_2O_2			hypophosphite	hypophosphito	
PHO_3			phosphite	phosphito	
PO_4			phosphate	phosphato	
AsO_4			arsenate	arsenato	
VO		vanadyl			
CO	carbon monoxide	carbonyl		carbonyl	carbonyl
CS		thiocarbonyl			
CH_3O	methoxyl		methanolate	methoxo	methoxy
C_2H_5O	ethoxyl		ethanolate	ethoxo	ethoxy
CH_3S			methanethiolate	methanethiolato	methylthio
C_2H_5S			ethanethiolate	ethanethiolato	ethylthio
CN		cyanogen	cyanide	cyano	cyano
OCN			cyanate	cyanato	cyanato
SCN			thiocyanate	thiocyanato and isothiocyanato	thiocyanato and isothiocyanato
SeCN			selenocyanate	selenocyanato	selenocyanato
TeCN			tellurocyanate	tellurocyanato	
CO_3			carbonate	carbonato	
HCO_3			hydrogen carbonate	hydrogen carbonato	
CH_3CO_2			acetate	acetato	acetoxy
CH_3CO	acetyl	acetyl			acetyl
C_2O_4			oxalate	oxalato	

[1] If necessary, oxidation state is to be given by Stock notation.

◆ Although some additions might be made to this list, especially in the last column, and a few changes suggested, no attempt has been made to do so at this time. *Cf.* comments at such rules as 3.31, 3.32, 5.35, 6.2, and 7.312.

ifications with Greek letters or with Roman numerals (α-iron, ice-I, *etc.*). The method is similar to the use of trivial names, and is likely to continue to be of use in the future in cases where the existence of polymorphism is established, but not the structures underlying it. Regrettably there has been no consistent system, and some investigators have designated as α the form stable at ordinary temperatures, while others have used α for the form stable immediately below the melting point, and some have even changed an already established usage and renamed α-quartz β-quartz, thereby causing confusion. If the α–β nomenclature is used for two substances A and B, difficulties are encountered when the binary system A–B is studied.

A rational system should be based upon crystal structure, and the designations α, β, γ, *etc.*, should be regarded as provisional, or as trivial names. The designations should be as short and understandable as possible, and convey a maximum of information to the reader. The rules suggested here have been framed as a basis for future work, and it is hoped that experience in their use may enable more specific rules to be formulated at a later date.

8.1.—For chemical purposes (*i.e.*, when particular mineral occurrences are not under consideration) polymorphs should be indicated by adding the crystal system after the name or formula. For example, zinc sulfide(cub.) or ZnS(cub.) corresponds to zinc blende or sphalerite, and ZnS(hex.) to wurtzite. The Commission considers that these abbreviations might with advantage be standardized internationally:

cub. = cubic
c. = body-centered
f. = face-centered
tetr. = tetragonal
o-rh. = orthorhombic
hex. = hexagonal
trig. = trigonal
mon. = monoclinic
tric. = triclinic

Slightly distorted lattices may be indicated by use of the *circa* sign, ∼. Thus, for example, a slightly distorted face-centered cubic lattice would be expressed as ∼f.cub.

8.2.—Crystallographers may find it valuable to add the space-group; it is doubtful whether this system would commend itself to chemists where 8.1 is sufficient.

8.3.—Simple well-known structures may also be designated by giving the type-compound in italics in parentheses; but this system often breaks down because many structures are not referable to a type in this way. Thus, AuCd above 70° may be written as AuCd(cub.) or as AuCd(*CsCl-type*); but at low temperature only as AuCd(o-rh.), as its structure cannot be referred to a type.

◆ *Cf.* 6.5 and 6.52.

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