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Richard M. Hartshorn, Karl-Heinz Hellwich, Andrey Yerin, Ture Damhus ...+1 more authors

Institutions: University of Canterbury, Advanced Chemistry Development, Novozymes, University of Cape Town

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IUPAC Technical Report

Richard M. Hartshorn*, Karl-Heinz Hellwich, Andrey Yerin, Ture Damhus and Alan T. Hutton

Brief guide to the nomenclature of inorganic chemistry

Abstract: This IUPAC Technical Report (PAC-REP-14-07-18) is one of a series that seeks to distil the essentials of IUPAC nomenclature recommendations. The present report provides a succinct summary of material presented in the publication *Nomenclature of Inorganic Chemistry – IUPAC Recommendations 2005*. The content of this report will be republished and disseminated as a four-sided lift-out document (see supplementary information) which will be available for inclusion in textbooks and similar publications.

Keywords: coordination chemistry; inorganic chemistry; nomenclature; organometallic chemistry.

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CONTENTS

Preamble	1040
1. Stoichiometric or compositional names	1040
2. Complexes and additive nomenclature	
2.1. Overall approach	1042
2.2. Central atom(s) and ligands	1042
2.3. Assembling additive names	1043
2.4. Specifying connectivity	1043
2.5. Bridging ligands	1044
2.6. Organometallic compounds	1044
2.7. Formulae of coordination compounds	1046
2.8. Inorganic oxoacids and related compounds	1047
3. Stereodescriptors	1048
4. Summary	1048
5. Membership of sponsoring body	1048
References	1049

Article note: Sponsoring body: IUPAC Division of Chemical Nomenclature and Structure Representation.

***Corresponding author: Richard M. Hartshorn**, Department of Chemistry, University of Canterbury, Private Bag 4800, Christchurch, New Zealand, e-mail: inorganic.nomenclature@iupac.org

Karl-Heinz Hellwich: Postfach 10 07 31, 63007 Offenbach, Germany

Andrey Yerin: Advanced Chemistry Development, Ul. Akademika Bakuleva, 6, Str. 1, RF-117513 Moscow, Russia

Ture Damhus: Novozymes A/S, Brudelysvej 32, 6BD1, DK-2880 Bagsvaerd, Denmark

Alan T. Hutton: Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa

Preamble

The universal adoption of an agreed chemical nomenclature is a key tool for communication in the chemical sciences, for computer-based searching in databases, and for regulatory purposes, such as those associated with health and safety or commercial activity. The International Union of Pure and Applied Chemistry (IUPAC) provides recommendations on the nature and use of chemical nomenclature [1]. The basics of this nomenclature are shown here, and in companion documents on the nomenclature systems for organic chemistry [2] and polymers [3], with hyperlinks to the original documents. An overall summary of chemical nomenclature can be found in *Principles of Chemical Nomenclature* [4]. Greater detail can be found in the *Nomenclature of Inorganic Chemistry*, colloquially known as the Red Book [5], and in the related publications for organic compounds (the Blue Book) [6] and polymers (the Purple Book) [7]. It should be noted that many compounds may have non-systematic or semi-systematic names (some of which are not accepted by IUPAC for several reasons, for example because they are ambiguous) and IUPAC rules allow for more than one systematic name in many cases. IUPAC is working towards identification of single names which are to be preferred for regulatory purposes (Preferred IUPAC Names, or PINs).

Note: In this document, the symbol '=' is used to split names that happen to be too long for the column format, unless there is a convenient hyphen already present in the name.

The boundaries between 'organic' and 'inorganic' compounds are blurred. The nomenclature types described in this document are applicable to compounds, molecules and ions that do not contain carbon, but also to many structures that do contain carbon (Section 2), notably those containing elements of Groups 1–12. Most boron-containing compounds are treated using a special nomenclature [8].

1 Stoichiometric or compositional names

A **stoichiometric** or **compositional** name provides information only on the composition of an ion, molecule, or compound, and may be related to either the empirical or molecular formula for that entity. It does not provide any structural information.

For **homoatomic entities**, where only one element is present, the name is formed (Table 1) by combining the element name with the appropriate **multiplicative prefix** (Table 2). Ions are named by adding charge numbers in parentheses, e.g., (1+), (3+), (2–), and for (most) homoatomic anion names 'ide' is added in place

Table 1: Examples of homoatomic entities.

Formula	Name	Formula	Name
O ₂	dioxygen	Cl [–]	chloride(1–) or chloride
S ₈	octasulfur	I ₃ [–]	triiodide(1–)
Na ⁺	sodium(1+)	O ₂ ^{2–}	dioxide(2–) or peroxide
Fe ³⁺	iron(3+)	N ₃ [–]	trinitride(1–) or azide

Table 2: Multiplicative prefixes for simple and complicated entities.

No.	Simple	Complicated	No.	Simple	Complicated
2	di	bis	8	octa	octakis
3	tri	tris	9	nona	nonakis
4	tetra	tetrakis	10	deca	decakis
5	penta	pentakis	11	undeca	undecakis
6	hexa	hexakis	12	dodeca	dodecakis
7	hepta	heptakis	20	icosa	icosakis

of the 'en', 'ese', 'ic', 'ine', 'ium', 'ogen', 'on', 'orus', 'um', 'ur', 'y' or 'ygen' endings of element names [9]. Exceptions include Zn and group 18 elements ending in 'on', where the 'ide' ending is added to the element names. For some elements (e.g., Fe, Ag, Au) a Latin stem is used before the 'ide' ending (*cf.* Section 2.3) [9]. Certain ions may have acceptable traditional names (used without charge numbers).

Binary compounds (those containing atoms of two elements) are named stoichiometrically by combining the element names and treating, by convention, the element reached first when following the arrow in the element sequence (Figure 1) as if it were an anion. Thus the name of this formally 'electronegative' element is given an 'ide' ending and is placed after the name of the formally 'electropositive' element followed by a space (Table 3).

Again, multiplicative prefixes (Table 2) are applied as needed, and certain acceptable alternative names [10] may be used. Stoichiometry may be implied in some cases by the use of oxidation numbers, but is often omitted for common cases, such as in calcium fluoride.

Heteropolyatomic entities in general can be named similarly using compositional nomenclature, but often either substitutive [11] or additive nomenclature (Section 2) is used. In the latter case information is also provided about the way atoms are connected. For example, POCl_3 (or PCl_3O , compositional name phosphorus trichloride oxide) is given an additive name in Table 10.

Certain ions have traditional short names, which are commonly used and are still acceptable (e.g., ammonium, NH_4^+ ; hydroxide, OH^- ; nitrite, NO_2^- ; phosphate, PO_4^{3-} ; diphosphate, $\text{P}_2\text{O}_7^{4-}$).

Inorganic compounds in general can be combinations of cations, anions and neutral entities. By convention, the name of a compound is made up of the names of its component entities: cations before anions and neutral components last (see examples in Table 4).

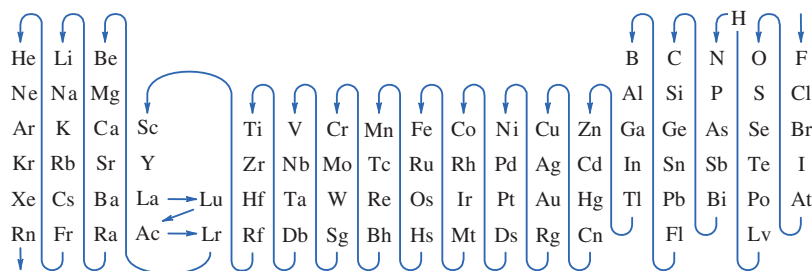


Figure 1: Element sequence.

Table 3: Examples of binary compounds.

Formula	Name	Formula	Name
GaAs	gallium arsenide	FeCl_2	iron dichloride or iron(II) chloride
CO_2	carbon dioxide	FeCl_3	iron trichloride or iron(III) chloride
CaF_2	calcium difluoride or calcium fluoride	H_2O_2	dihydrogen dioxide or hydrogen peroxide

Table 4: Use of multiplicative prefixes in compositional names.

Formula	Name
$\text{Ca}_3(\text{PO}_4)_2$	tricalcium bis(phosphate)
$\text{Ca}_2\text{P}_2\text{O}_7$	dicalcium diphosphate
BaO_2	barium(2+) dioxide(2-) or barium peroxide
$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$	magnesium sulfate heptahydrate
$\text{CdSO}_4 \cdot 6\text{NH}_3$	cadmium sulfate—ammonia (1/6)
$\text{AlK}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	aluminium potassium bis(sulfate)—water (1/12) or aluminium potassium bis(sulfate) dodecahydrate
$\text{Al}_2(\text{SO}_4)_3 \cdot \text{K}_2\text{SO}_4 \cdot 24\text{H}_2\text{O}$	dialuminium tris(sulfate)—dipotassium sulfate—water (1/1/24)

The number of each entity present has to be specified in order to reflect the composition of the compound. For this purpose multiplicative prefixes (Table 2) are added to the name of each entity. The prefixes are ‘di’, ‘tri’, ‘tetra’, etc., for use with names for simple entities, or ‘bis()’, ‘tris()’, ‘tetrakis()’, etc., for names for most entities which themselves contain multiplicative prefixes or locants. Care must also be taken in situations when use of a simple multiplicative prefix may be misinterpreted, e.g., tris(iodide) must be used for 3I^- rather than triiodide (which is used for I_3^-), and bis(phosphate) rather than diphosphate (which is used for $\text{P}_2\text{O}_7^{4-}$). Examples are shown in Table 4. There is no elision of vowels (e.g., tetraaqua, pentaoxide), except in the special case of monoxide.

Names of neutral components are separated by ‘em’ dashes without spaces. Inorganic compounds may themselves be components in (formal) **addition compounds** (last four examples in Table 4). The ratios of component compounds can be indicated, in general, using a stoichiometric descriptor in parentheses after the name (see the last three examples in Table 4). In the special case of hydrates, multiplicative prefixes can be used with the term ‘hydrate’.

2 Complexes and additive nomenclature

2.1 Overall approach

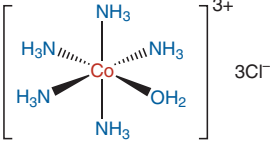
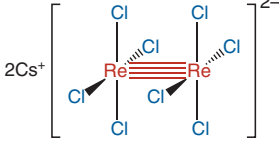
Additive nomenclature was developed in order to describe the structures of coordination entities, or complexes, but this method is readily extended to other molecular entities as well. Mononuclear complexes are considered to consist of a central atom, often a metal ion, which is bonded to surrounding small molecules or ions, which are referred to as ligands. The names of complexes are constructed (Table 5) by adding the names of the ligands *before* those of the central atoms, using appropriate multiplicative prefixes. Formulae are constructed by adding the symbols or abbreviations of the ligands *after* the symbols of the central atoms (Section 2.7).

2.2 Central atom(s) and ligands

The first step is to identify the central atom(s) and thereby also the ligands. By convention, the electrons involved in bonding between the central atom and a ligand are usually treated as belonging to the ligand (and this will determine how it is named).

Each ligand is named as a separate entity using appropriate nomenclature [4] – usually substitutive nomenclature for organic ligands [2, 4, 6] and additive nomenclature for inorganic ligands. A small number of common molecules and ions are given **special names** when present in complexes. For example, a water ligand is represented in the full name by the term ‘aqua’. An ammonia ligand is represented by ‘ammine’,

Table 5: Producing names for complexes: simple ligands.

Structure to be named		
Central atom(s)	cobalt(III)	2 × rhenium
Identify and name ligands	ammonia → ammine water → aqua	chloride → chlorido
Assemble name	pentaammineaqua cobalt(III) chloride	caesium bis(tetrachloridorhenate)(Re–Re)(2–)

while carbon monoxide bound to the central atom through the carbon atom is represented by the term ‘carbonyl’ and nitrogen monoxide bound through nitrogen is represented by ‘nitrosyl’. Names of **anionic ligands** that end in ‘ide’, ‘ate’, or ‘ite’ are modified within the full additive name for the complex to end in ‘ido’, ‘ato’, or ‘ito’, respectively. Note that the ‘ido’ ending is now used for halide and oxide ligands as well. By convention, a single coordinated hydrogen atom is always considered anionic and it is represented in the name by the term ‘hydrido’, whereas coordinated dihydrogen is usually treated as a neutral two-electron donor entity.

2.3 Assembling additive names

Once the ligands have been named, the name can be assembled. This is done by listing the ligand names in alphabetical order before the name of the central atom(s), *without regard* to ligand charge.

If there is more than one ligand of a particular kind bound to a central atom in the same way, the number of such identical ligands is indicated using the appropriate multiplicative prefix for simple or complicated ligands (Table 2), not changing the already established alphabetical order of ligands. The nesting order of enclosing marks, for use in names where more than one set of enclosing marks is required, is: (), [], {}, etc.

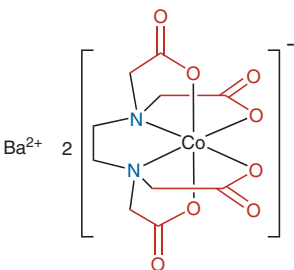
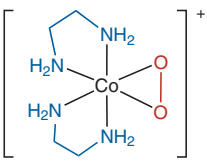
Any **metal-metal bonds** are indicated by placing the central atom symbols in parentheses, in italics and connected by an ‘em’ dash, after the name of the complex (without spaces). The **charge number** of the complex or the **oxidation number** of the central atom is appended to the name of the complex. For **anions** that are named additively, the name of the central atom is given the ‘ate’ ending in a similar way to the ‘ide’ endings of homoatomic anions (Section 1). In some cases, by tradition, the Latin stem is used for the ‘ate’ names, such as in ferrate (for iron), cuprate (for copper), argentate (for silver), stannate (for tin), aurate (for gold), and plumbate (for lead) [12]. Finally, the rules of compositional nomenclature (Section 1) are used to combine the additive names of ionic or neutral coordination entities with the names of any other entities that are part of the compound.

2.4 Specifying connectivity

Some ligands can bind to a central atom through different atoms under different circumstances. Specifying just which ligating (coordinating) atoms are bound in any given complex can be achieved by adding **κ -terms** to the name of the ligand. The κ -term comprises the Greek letter κ followed by the italicised element symbol of the ligating atom. For more complicated ligands, the κ -term is often placed within the ligand name following the group to which the κ -term refers. Multiple identical links to a central atom can be indicated by the addition of the appropriate numeral as a superscript between the κ and element symbols (see Table 6). These possibilities are discussed in more detail in the Red Book [13]. If the ligating atoms of a ligand are contiguous (i.e., directly bonded to one another), then an **η -term** is used instead, for example, for many organometallic compounds (Section 2.6) and the peroxido complex in Table 6.

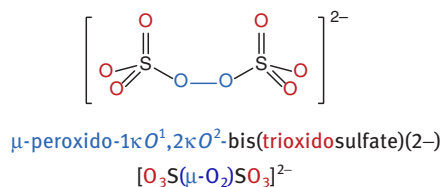
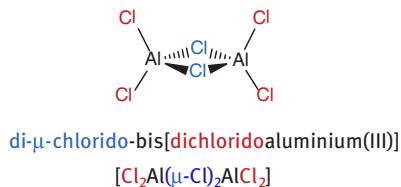
A κ -term is required for ligands where more than one coordination mode is possible. Typical cases are thiocyanate, which can be bound through either the sulfur atom (thiocyanato- κ S) or the nitrogen atom (thiocyanato- κ N), and nitrite, which can be bound through either the nitrogen atom (M-NO₂, nitrito- κ N) or an oxygen atom (M-ONO, nitrito- κ O). The names pentaammine(nitrito- κ N)cobalt(2+) and pentaammine(nitrito- κ O)cobalt(2+) are used for each of the isomeric nitrito complex cations. More examples of constructing names using κ -terms to specify the connectivity of ligands are shown in Table 6. A κ -term may also be used to indicate to which central atom a ligand is bound if there is more than one central atom (Section 2.5).

Table 6: Producing names for complexes: complicated ligands.

Structure to be named		
		
Central atom	cobalt(III) → cobaltate(III)	platinum(II)
Identify and name ligands	2,2',2'',2'''-(ethane-1,2-diyldinitrilo)=tetraacetato → 2,2',2'',2'''-(ethane-1,2-diyldinitrilo)tetraacetato	chloride → chlorido triphenylphosphane
Specify ligating atoms	2,2',2'',2'''-(ethane-1,2-diyldinitrilo-κ ² N)=tetraacetato-κ ⁴ O	<i>not required for chloride</i> triphenylphosphane-κP
Assemble name	barium [2,2',2'',2'''-(ethane-1,2-diyldinitrilo-κ ² N)tetraacetato-κ ⁴ O]cobaltate(III)	dichloridobis(triphenylphosphane-κP)=platinum(II)
Structure to be named		
		
Central atom	cobalt(III)	molybdenum(III)
Identify and name ligands	ethane-1,2-diamine peroxide → peroxido	chloride → chlorido 1,4,8,12-tetrathiacyclopentadecane
Specify ligating atoms	ethane-1,2-diamine-κ ² N η ² -peroxido	<i>not required for chloride</i> 1,4,8,12-tetrathiacyclopentadecane-κ ³ S ¹ , S ⁴ , S ⁸
Assemble name	bis(ethane-1,2-diamine-κ ² N)(η ² -peroxido)=cobalt(III)	trichlorido(1,4,8,12-tetrathiacyclopentadecane-κ ³ S ¹ , S ⁴ , S ⁸)molybdenum(III)

2.5 Bridging ligands

Bridging ligands are those bound to more than one central atom. They are differentiated in names by the addition of the prefix 'μ' (Greek mu), with the prefix and the name of the bridging ligand being separated from each other, and from the rest of the name, by hyphens. This is sufficient if the ligand is monoatomic, but if the ligand is more complicated it may be necessary to specify which ligating atom of the ligand is attached to which central atom. This is certainly the case if the ligating atoms are of different kinds, and κ-terms can be used for this purpose.



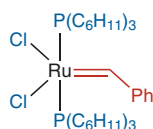
2.6 Organometallic compounds

Organometallic compounds contain at least one bond between a metal atom and a carbon atom. They are named as coordination compounds, using the additive nomenclature system (see above).

The name for an organic ligand **binding through one carbon atom** may be derived either by treating the ligand as an anion or as a neutral substituent group. The compound $[\text{Ti}(\text{CH}_2\text{CH}_2\text{CH}_3)_3\text{Cl}_3]$ is thus named as **trichlorido(propan-1-ido)titanium** or as **trichlorido(propyl)titanium**. Similarly, ‘methanido’ or ‘methyl’ may be used for the ligand $-\text{CH}_3$.

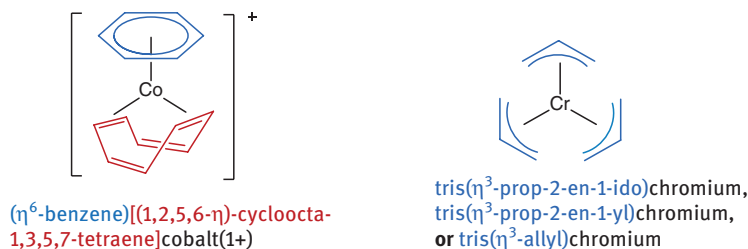
When an organic ligand forms **two or three metal-carbon single bonds** (to one or more metal centres), the ligand may be treated as a di- or tri-anion, with the endings ‘diido’ or ‘triido’ being used, with no removal of the terminal ‘e’ of the name of the parent hydrocarbon. Again, names derived by regarding such ligands as substituent groups and using the suffixes ‘diyl’ and ‘triyl’ are still commonly encountered. Thus, the bidentate ligand $-\text{CH}_2\text{CH}_2\text{CH}_2-$ would be named propane-1,3-diido (or propane-1,3-diyl) when chelating a metal centre, and μ -propane-1,3-diido (or μ -propane-1,3-diyl) when bridging two metal atoms.

Organometallic compounds containing a **metal-carbon multiple bond** are given substituent prefix names derived from the parent hydrides which end with the suffix ‘ylidene’ for a metal-carbon double bond and with ‘ylidyne’ for a triple bond. These suffixes either replace the ending ‘ane’ of the parent hydride, or, more generally, are added to the name of the parent hydride with the insertion of a locant and the elision of the terminal ‘e’, if present. Thus, the entity $\text{CH}_3\text{CH}_2\text{CH}=\text{}$ as a ligand is named propylidene and $(\text{CH}_3)_2\text{C}=\text{}$ is called propan-2-ylidene. The ‘diido’/‘triido’ approach, outlined above, can also be used in this situation. The terms ‘carbene’ and ‘carbyne’ are not used in systematic nomenclature.



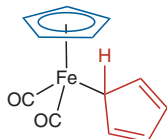
dichlorido(phenylmethylidene)bis(tricyclohexylphosphane-κP)ruthenium,
dichlorido(phenylmethanediido)bis(tricyclohexylphosphane-κP)ruthenium,
or (benzylidene)dichloridobis(tricyclohexylphosphane-κP)ruthenium

The special nature of the bonding to metals of unsaturated hydrocarbons in a ‘side-on’ fashion *via* their π -electrons requires the **eta (η) convention**. In this ‘hapto’ nomenclature, the number of *contiguous* atoms in the ligand coordinated to the metal (the hapticity of the ligand) is indicated by a right superscript on the eta symbol, e.g., η^3 (‘eta three’ or ‘trihapto’). The η -term is added as a prefix to the ligand name, or to that portion of the ligand name most appropriate to indicate the connectivity, with locants if necessary.



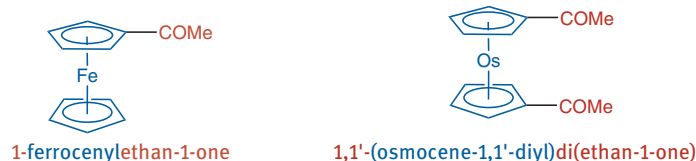
A list of many **π -bonding unsaturated ligands**, neutral and anionic, can be found in the Red Book [14].

Note that the ubiquitous ligand $\eta^5\text{-C}_5\text{H}_5$, strictly η^5 -cyclopenta-2,4-dien-1-ido, is also acceptably named η^5 -cyclopentadienido or η^5 -cyclopentadienyl. When cyclopenta-2,4-dien-1-ido coordinates through one carbon atom *via* a σ bond, a κ -term is added for explicit indication of that bonding. The symbol η^1 should not be used, as the eta convention applies only to the bonding of contiguous atoms in a ligand.



dicarbonyl(η^5 -cyclopentadienido)(cyclopenta-2,4-dien-1-ido-κC¹)iron
or dicarbonyl(η^5 -cyclopentadienyl)(cyclopenta-2,4-dien-1-yl-κC¹)iron

Discrete molecules containing two *parallel* η^5 -cyclopentadienido ligands in a ‘sandwich’ structure around a transition metal, as in bis(η^5 -cyclopentadienido)iron, $[\text{Fe}(\eta^5\text{-C}_5\text{H}_5)_2]$, are generically called **metallocenes** and may be given ‘ocene’ names, in this case ferrocene. These ‘ocene’ names may be used in the same way as parent hydride names are used in substitutive nomenclature, with substituent group names taking the forms ‘ocenyl’, ‘ocenediyl’, ‘ocenetriyl’ (with insertion of appropriate locants).



By convention, ‘organoelement’ compounds of the **main group elements** are named by substitutive nomenclature if derived from the elements of Groups 13–16, but by additive nomenclature if derived from the elements of Groups 1 and 2. In some cases compositional nomenclature is used if less structural information is to be conveyed. More detail is provided in the Red Book [15].

2.7 Formulae of coordination compounds

Line formulae for coordination entities are constructed within square brackets to specify the composition of the entity. The overall process is shown in Table 7. The symbol for the central atom is placed first and is then followed by the symbols or abbreviations for the ligands (in alphabetical order according to the way they are presented in the formula). Where possible the coordinating (ligating) atom should be placed nearer the central atom in order to provide more information about the structure of the complex. If possible, bridging ligands should be placed between central atom symbols for this same reason (see examples in Section 2.5). Generally ligand formulae and abbreviations are placed within enclosing marks (unless the ligand contains only one atom), remembering that square brackets are reserved to define the coordination sphere. Multiple ligands are indicated by a right subscript following the enclosing marks or ligand symbol.

Table 7: Producing line formulae for complexes.

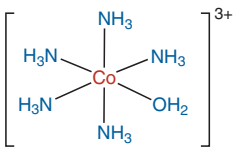
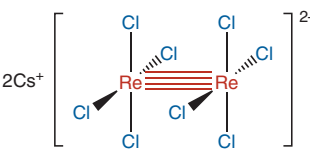
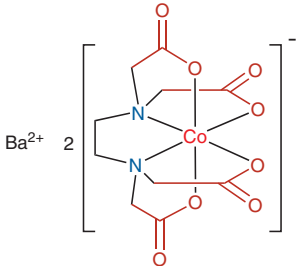
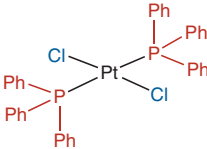
Structure		
Central atom(s)	Co	2 × Re
Ligands	NH ₃ , OH ₂	Cl
Assemble formula	$[\text{Co}(\text{NH}_3)_5(\text{OH}_2)]\text{Cl}_3$	$\text{Cs}_2[\text{Cl}_4\text{ReReCl}_4]$
Structure		
Central atom(s)	Co	Pt
Abbreviate ligands	2,2',2'',2'''-(ethane-1,2-diyl)= dinitrilotetraacetate → edta	Cl triphenylphosphane → PPh ₃
Assemble formula	$\text{Ba}[\text{Co}(\text{edta})]_2$	$[\text{PtCl}_2(\text{PPh}_3)_2]$

Table 8: Examples of inorganic oxoacids and derivatives.

Formula	Traditional or organic name	Additive name
H_2SO_4 or $[\text{S}(\text{O})_2(\text{OH})_2]$	sulfuric acid	dihydroxidodioxidosulfur
$(\text{CH}_3)_2\text{SO}_4$ or $[\text{S}(\text{O})_2(\text{OMe})_2]$	dimethyl sulfate	dimethoxidodioxidosulfur or dimethanolatodioxidosulfur
H_2PHO_3 or $[\text{P}(\text{H})(\text{O})(\text{OH})_2]$	phosphonic acid*	hydridodihydroxidooxidophosphorus
$\text{PhP}(\text{O})(\text{OH})_2$	phenylphosphonic acid	dihydroxidooxido(phenyl)phosphorus

*The term ‘phosphorous acid’ has been used in the literature for both the species named phosphonic acid in Table 8 and that with the formula $\text{P}(\text{OH})_3$, trihydroxidophosphorus. It is used in organic nomenclature in the latter sense.

2.8 Inorganic oxoacids and related compounds

Inorganic oxoacids, and the anions formed by removing the acidic **hydrons** (H^+) from them, have traditional names, many of which are well-known and can be found in many textbooks: sulfuric acid, sulfate; nitric acid, nitrate; nitrous acid, nitrite; phosphoric acid, phosphate; arsenic acid, arsenate; arsine acid, arsinite; silicic acid, silicate; etc. These names are retained in IUPAC nomenclature, firstly because they almost invariably are the names used in practice, and secondly because they play a special role in organic nomenclature when names are needed for organic derivatives. However, all the oxoacids themselves and their derivatives may be viewed as coordination entities and named systematically using additive nomenclature (Table 8) [16].

The traditional oxoacid names may be modified according to established rules for naming derivatives formed by **functional replacement** [16]: thus ‘thio’ denotes replacement of $=\text{O}$ by $=\text{S}$; prefixes ‘fluoro’, ‘chloro’, etc., and infixes ‘fluorid’, ‘chlorid’, etc., denote replacement of $-\text{OH}$ by $-\text{F}$, $-\text{Cl}$, etc.; ‘peroxy’/‘peroxo’ denote replacement of $-\text{O}-$ by $-\text{OO}-$; and so forth (Table 9).

If all hydroxy groups in an oxoacid are replaced, the compound is no longer an acid and is not named as such, but will have a traditional **functional class name** [16] as, e.g., an acid halide or amide. Such compounds may again be systematically named using additive nomenclature (Table 10).

A special construction is used in **hydrogen names**, which allows the indication of hydrons bound to an anion without specifying exactly where. In such names, the word ‘hydrogen’ is placed at the front of the name with a multiplicative prefix (if applicable) and with no space between it and the rest of the name, which is placed in parentheses. For example, dihydrogen(diphosphate)(2-) denotes $\text{H}_2\text{P}_2\text{O}_7^{2-}$, a diphosphate ion to which two hydrons have been added, with the positions not known or at least not being specified.

One may view the common names for partially dehydrated oxoacids, such as hydrogenphosphate, HPO_4^{2-} , and dihydrogenphosphate, H_2PO_4^- , as special cases of such hydrogen names. In these simplified names, the charge number and the parentheses around the main part of the name are left out. Again, these particular anions may be named systematically by additive nomenclature. The word ‘hydrogen’ is placed *separately* in

Table 9: Examples of derivatives of inorganic oxoacids and anions formed by functional replacement.

Formula	Name indicating functional replacement	Additive name
H_3PS_4 or $[\text{P}(\text{S})(\text{SH})_3]$	tetrathiophosphoric acid or phosphorotetrathioic acid	tris(sulfanido)sulfidophosphorus
H_2PFO_3 or $[\text{PF}(\text{O})(\text{OH})_2]$	fluorophosphoric acid or phosphorofluoridic acid	fluoridodihydroxidooxidophosphorus
$\text{S}_2\text{O}_3^{2-}$ or $[\text{S}(\text{O})_3(\text{S})]^{2-}$	thiosulfate or sulfurothioate	trioxidosulfidosulfate(2-)
$[\text{O}_3\text{S}(\mu\text{-O}_2)\text{SO}_3]^{2-}$	peroxydisulfate	see Section 2.5

Table 10: Examples of functional class names and corresponding additive names.

Formula	Functional class name	Additive name
PCl_3O	phosphoryl trichloride	trichloridooxidophosphorus
SOCl_2	sulfuryl dichloride	dichloridodioxidosulfur
$\text{S}(\text{NH}_2)_2\text{O}_2$	sulfuric diamide	diamidodioxidosulfur

forming analogous names in organic nomenclature, for example, dodecyl hydrogen sulfate, $\text{C}_{12}\text{H}_{25}\text{OS}(\text{O})_2\text{OH}$. This difference between the two systems has the consequence that the important carbon-containing ion HCO_3^- can be named equally correctly as ‘hydrogen carbonate’ and as ‘hydrogencarbonate’ (but not as bicarbonate).

3 Stereodescriptors

The approximate geometry around the central atom is described using a **polyhedral symbol** placed in front of the name. The symbol is made up of italicised letter codes for the geometry and a number that indicates the coordination number. Frequently used polyhedral symbols are *OC*-6 (octahedral), *SP*-4 (square-planar), *T*-4 (tetrahedral), *SPY*-5 (square-pyramidal), and *TBPY*-5 (trigonal-bipyramidal). More complete lists are available [17].

The relative positions of ligating groups around a central atom can be described using a **configuration index** that is determined in a particular way for each geometry [18], based on the Cahn–Ingold–Prelog priorities of the ligating groups [19, 20], and it may change if the ligands change, even if the geometry remains the same. The absolute configuration can also be described. Generally configuration indices are used only if there is more than one possibility and a particular stereoisomer is to be identified. The full stereodescriptors for the particular square-planar platinum complexes shown below are (*SP*-4-2) and (*SP*-4-1), for the *cis* and *trans* isomers, respectively. Alternatively, a range of traditional stereodescriptors may be used in particular situations. Thus the isomers that are possible when a square-planar centre is coordinated by two ligating groups of one type and two of another are referred to as *cis*- (when the identical ligands are coordinated next to each other) or *trans*- (when they are coordinated opposite to each other).



Octahedral centres with four ligands of one kind and two of another can also be referred to as *cis*- (when the two identical ligands are coordinated next to each other) or *trans*- (when they are coordinated opposite each other). Octahedral centres with three of each of two kinds of ligand can be described as *fac*- (facial), when the three ligands of a particular kind are located at the corners of a face of the octahedron, or *mer*- (meridional), when they are not.

4 Summary

This document provides an outline of the essential nomenclature rules for producing names and formulae for inorganic compounds, coordination compounds, and organometallic compounds. The complementary document for nomenclature systems of organic chemistry [2] will also be useful to the reader.

Names and formulae have only served half their role when they are created and used to describe or identify compounds, for example, in publications. Achieving their full role requires that the reader of a name or formula is able to interpret it successfully, for example, to produce a structural diagram. The present document is also intended to assist in the interpretation of names and formulae.

Finally, we note that IUPAC has produced recommendations on the graphical representation of chemical structures and their stereochemical configurations [21, 22].

5 Membership of sponsoring body

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