

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.

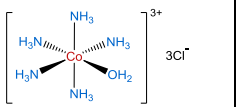
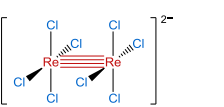
Names of neutral components are separated by ‘em’ dashes without spaces. Inorganic compounds may themselves be components in (formal) **addition compounds** (last four examples in Table 4). The ratios of component compounds can be indicated, in general, using a stoichiometric descriptor in parentheses 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).

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(tetrachlorido= rhenate)(Re—Re)(2-)

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 nomenclature⁴ – 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’, 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.*

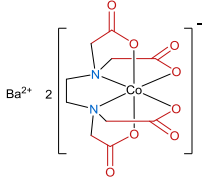
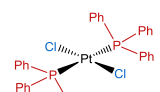
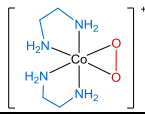
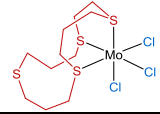
Any **metal-metal bonds** are indicated by placing the central atom symbols in parentheses, in italics and connected by an ‘em’ dash, after the name of the complex (without spaces). The **charge number** of the complex or the **oxidation number** of the central atom is appended to the name of the complex. 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 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-κS) or the nitrogen atom (thiocyanato-κN), and nitrite, which can be bound through either the nitrogen atom (M–NO₂, nitrito-κN), or an oxygen atom (M–ONO, nitrito-κO). The names pentaammine(nitrito-κN)cobalt(2+) and pentaammine(nitrito-κO)cobalt(2+) are used for

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-diyl=dinitrilo)tetraacetate → 2,2',2'',2'''-(ethane-1,2-diyl=dinitrilo)tetraacetato	chloride → chlorido triphenylphosphane
Specify ligating atoms	2,2',2'',2'''-(ethane-1,2-diyl=dinitrilo-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-diyl)dinitrilo-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-κ³S¹,S⁴,S⁸
Assemble name	bis(ethane-1,2-diamine-κ²N)= (η²-peroxido)cobalt(III)	trichlorido(1,4,8,12-tetrathiacyclopentadecane-κ³S¹,S⁴,S⁸)molybdenum(III)

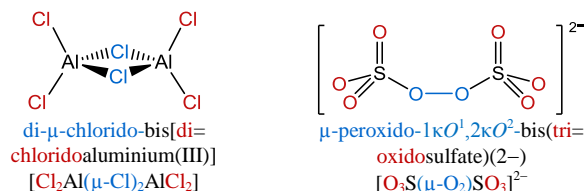
¹² Reference 5, Table X.

¹³ Reference 5, Section IR-9.2.4.

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).

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.



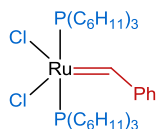
2.6 Organometallic compounds

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 [Ti(CH₂CH₂CH₃)Cl₃] is thus named as **trichlorido(propan-1-ido)titanium** or as **trichlorido(propyl)titanium**. Similarly, ‘methanido’ or ‘methyl’ may be used for the ligand –CH₃.

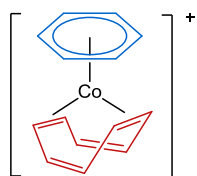
When an organic ligand forms **two or three metal-carbon single bonds** (to one or more metal centres), the ligand may be treated as a di- or tri-anion, with the endings ‘diido’ or ‘triido’ being used, with no removal of the terminal ‘e’ of the name of the parent hydrocarbon. Again, names derived by regarding such ligands as substituent groups and using the suffixes ‘diyl’ and ‘triyl’ are still commonly encountered. Thus, the bidentate ligand –CH₂CH₂CH₂– 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 insertion of a locant and elision of the terminal ‘e’, if present. Thus, the entity CH₃CH₂CH= as a ligand is named propylidene and (CH₃)₂C= 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.

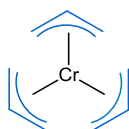


dichlorido(phenylmethylidene)bis(tricyclohexylphosphane- κ P)ruthenium,
dichlorido(phenylmethanediido)bis(tricyclohexylphosphane- κ P)ruthenium,
or (benzylidene)dichloridobis(tricyclohexylphosphane- κ P)ruthenium

The special nature of the bonding to metals of unsaturated hydrocarbons in a ‘side-on’ fashion *via* their π -electrons requires



(η^6 -benzene)[(1,2,5,6- η)-cycloocta-1,3,5,7-tetraene]cobalt(1+)

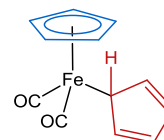


tris(η^3 -prop-2-en-1-ido)chromium,
tris(η^3 -prop-2-en-1-yl)chromium,
or tris(η^3 -allyl)chromium

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.

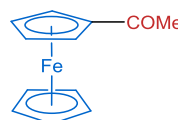
A list of many **π -bonding unsaturated ligands**, neutral and anionic, can be found in the Red Book.¹⁴

Note that the ubiquitous ligand η^5 -C₅H₅, 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.

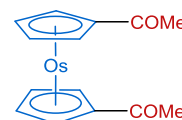


dicarbonyl(η^5 -cyclopentadienido)(cyclopenta-2,4-dien-1-ido- κ C¹)iron
or dicarbonyl(η^3 -cyclopentadienyl)(cyclopenta-2,4-dien-1-yl- κ C¹)iron

Discrete molecules containing two *parallel* η^5 -cyclopentadienido ligands in a ‘sandwich’ structure around a transition metal, as in bis(η^5 -cyclopentadienido)iron, [Fe(η^5 -C₅H₅)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).



1-ferrocenylethan-1-one



1,1'-(osmocene-1,1'-diyl)di-(ethan-1-one)

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

Table 7: Producing line formulae for complexes

Structure		
Central atom(s)	Co	2 × Re
Ligands	NH ₃ , OH ₂	Cl
Assemble formula	[Co(NH ₃) ₅ (OH ₂)]Cl ₃	Cs ₂ [Cl ₄ ReReCl ₄]
Structure		
Central atom(s)	Co	Pt
Abbreviate ligands	2,2',2'',2'''-(ethane-1,2-diyl)dinitrilo)tetraacetate → edta	Cl triphenylphosphane → PPh ₃
Assemble formula	Ba[Co(edta)] ₂	[PtCl ₂ (PPh ₃) ₂]

¹⁴ Reference 5, Table IR-10.4.

¹⁵ Reference 5, Section IR-10.3.

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.

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

Table 8: Examples of inorganic oxoacids and derivatives

Formula	Traditional or organic name	Additive name
H_2SO_4 or $[S(O)_2(OH)_2]$	sulfuric acid	dihydroxidodioxidosulfur
$(CH_3)_2SO_4$ or $[S(O)_2(OMe)_2]$	dimethyl sulfate	dimethoxidodioxidosulfur or dimethanolatodioxidosulfur
$H_2P(O)_3$ or $[P(H)(O)(OH)_2]$	phosphonic acid*	hydridodihydroxidooxido=phosphorus
$PhP(O)(OH)_2$	phenylphosphonic acid	dihydroxidooxido(phenyl)=phosphorus

*Note: 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 $P(OH)_3$, trihydroxidophosphorus. It is used in organic nomenclature in the latter sense.

The traditional oxoacid names may be modified according to established rules for naming derivatives formed by **functional replacement**¹⁶: thus 'thio' denotes replacement of =O by =S; prefixes 'fluoro', 'chloro', *etc.*, and infixes 'fluorid', 'chlorid', *etc.*, denote replacement of -OH by -F, -Cl, *etc.*; 'peroxy'/'peroxo' denote replacement of -O- by -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 $H_2P_2O_7^{2-}$, 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

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 $[P(S)(SH)_3]$	tetrathiophosphoric acid or phosphorotetrathioic acid	tris(sulfanido)sulfido=phosphorus
H_2PFO_3 or $[PF(O)(OH)_2]$	fluorophosphoric acid or phosphorofluoric acid	fluoridodihydroxido=oxidophosphorus
$S_2O_3^{2-}$ or $[S(O)_2(S)]^{2-}$	thiosulfate or sulfurothioate	trioxidosulfido=sulfate(2-)
$[O_3S(\mu-O_2)SO_3]^{2-}$	peroxydisulfate	see Section 2.5

¹⁶ Reference 5, Chapter IR-8.

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

Formula	Functional class name	Additive name
PCl_3O	phosphoryl trichloride	trichloridooxido=phosphorus
SCl_2O_2	sulfuryl dichloride	dichloridodioxidosulfur
$S(NH_2)_2O_2$	sulfuric diamide	diamidodioxidosulfur

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 forming analogous names in organic nomenclature, for example, dodecyl hydrogen sulfate, $C_{12}H_{25}OS(O)_2OH$. 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 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).



cis-diammine dichloridoplatinum(II)

trans-diammine dichloridoplatinum(II)

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.²⁰

¹⁷ Reference 4, Table P5; Reference 5, Tables IR-9.2 and IR-9.3.

¹⁸ Reference 5, Section IR-9.3.3.

¹⁹ R. S. Cahn, C. Ingold, V. Prelog, *Angew. Chem., Int. Ed. Engl.*, **5**, 385–415 and 511 (1966); V. Prelog, G. Helmchen, *Angew. Chem., Int. Ed. Engl.*, **21**, 567–583 (1982).

²⁰ J. Brecher, K. N. Degtyarenko, H. Gottlieb, R. M. Hartshorn, G. P. Moss, P. Murray-Rust, J. Nyitrai, W. Powell, A. Smith, S. Stein, K. Taylor, W. Town, A. Williams, A. Yerin, *Pure Appl. Chem.*, **78**(10), 1897–1970 (2006); J. Brecher, K. N. Degtyarenko, H. Gottlieb, R. M. Hartshorn, K.-H. Hellwich, J. Kahovec, G. P. Moss, A. McNaught, J. Nyitrai, W. Powell, A. Smith, K. Taylor, W. Town, A. Williams, A. Yerin, *Pure Appl. Chem.*, **80**(2), 277–410 (2008).

