P-69 Nomenclature of organometallic compounds

P-69.0 Introduction

This Section is partly an application of the principles, rules, and conventions established in previous Chapters, and partly an extension of these principles, rules, and conventions to reconcile the nomenclatures of organic and inorganic compounds (see ref 14) to name organometallic compounds.

Organometallic compounds traditionally are compounds having bonds between one or more metal atoms and one or more carbon atoms of an organic residue. In addition to the traditional metals and semimetals, some compounds containing elements such as boron, silicon, arsenic and selenium have sometimes been considered to be organometallic.

Metals and semimetals are divided into three categories: (1) those belonging to Groups 1 and 2, (2) those belonging to Goups 3-12 (transition metals) and (3) metals and semimetals of Groups 13 through 16. Thus a great part of nomenclature of organometallic compounds is outside the scope of this book covering organic compounds; it follows the principles, rules and conventions of the nomenclature of inorganic compounds described in the Nomenclature of Inorganic Chemistry (Red Book), in particular, Chapter I-10.9 (ref. 14).

All organometallic compounds can be named by a type of additive nomenclature conveniently called coordination nomenclature, a system in which the names of compounds are formed by adding the name(s) of (a) ligand(s), in alphanumerical order if there is more than one, to that of a central atom. (ref. 14., Chapters I-7, I-9). In formulas for compounds named by coordination nomenclature, the whole coordination entity of a neutral coordination compound is enclosed in brackets.

In this Chapter, only organometallic compounds involving the metal atoms of Groups 13, 14, 15, and 16 are considered, and preferred IUPAC names are noted for these. Organometallic compounds of the transition elements included in this Section are restricted to those with ligands attached through one or more carbon atoms; organometallic compounds with other ligating atoms are not a part of the discussion. Metallacycles and 'ocene' compounds are included. For organometallic compounds of the transition elements, preferred IUPAC names are not noted; neither are preselected names given (see P-12). This determination will await consideration by a task group on organometallic nomenclature.

P-69.1 Organometallic compounds of Groups 13, 14, 15, and 16

Organometallic compounds derived from elements of Groups 13, 14, 15, and 16 are named substitutively by prefixing the appropriate substituent names to the name of a parent hydride; they are the preferred IUPAC names.

Examples:

$Al(CH_2\text{-}CH_3)_3$

triethylalumane (PIN; substitutive name)
triethylaluminium (additive, coordination-type name)

$Pb(CH_2\text{-}CH_3)_4$

tetraethylplumbane (PIN; substitutive name)
tetraethyllead (additive, coordination-type name)

$BrSb(CH{=}CH_2)_2$

bromodiethenylstibane (PIN; substitutive name)
bromidodiethenidoantimony (coordination-type name)

$HIn(CH_3)_2$

dimethylindigane (PIN; sbstitutive name)
hydridodimethanidoindium (coordination-type name)

P-69.2 Organometallic compounds of elements in Groups 3 through 12

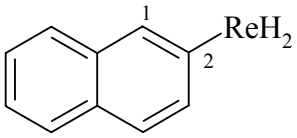
P-69.2.1 Coordination nomenclature is the main nomenclature method used to name organometallic compounds containing elements of Groups 3-12. It is described in *Nomenclature of Inorganic Chemistry* (ref. 14, Chapter 10) and in 'Nomenclature of organometallic compounds of the transition elements' (ref 24) It is discussed briefly and exemplified in this Section. The metal is always the central atom.

Linear formulae are composed of the symbol of the central atom, followed by the ligands, in alphabetical order if more than one is present. [This is a change from that described in the 1990 Inorganic Nomenclature recommendations (ref 14)]**.** In a line formula, a coordination entity is always placed in square brackets. No brackets are indicated when the structure is based on developed organic formulas.

P-69.2.2 Compounds consisting solely of individual metal atoms joined to a carbon atom of one or more organyl substituent groups and/or to one or more hydrogen atoms are named by citing the names of such organic groups or hydrogen in alphanumerical order, followed by the name of the metal. The presence of hydrogen attached to a metal atom must always be indicated by the prefix 'hydrido'.

Examples:

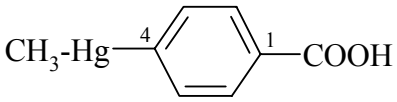
$[Hg\text{-}CH_3]^+$	$[Zn(CH_3)_2]$
methylmercury(1+)	dimethylzinc



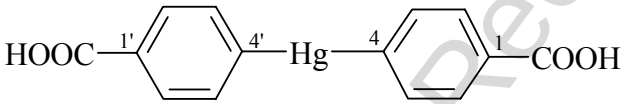
dihydrido(naphthalen-2-yl)rhenium

[Cu-C≡C-CH3]

(prop-1-yn-1yl)copper



(4-carboxyphenyl)methylmercury

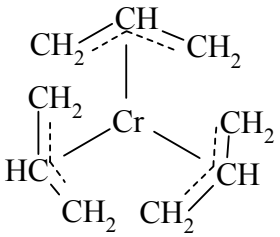


bis(4-carboxyphenyl)mercury

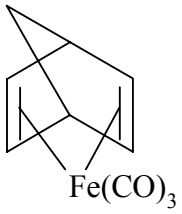
P-69.2.3 Organometallic groups with multicenter bonding to carbon atoms

In order to indicate multicenter bonding to carbon atoms, for example in an unsaturated system, the name of the ligand is preceded by the prefix η (eta) A right superscript is added to the symbol η to indicate the number of atoms that bind to the metal. When it is necessary to indicate that all unsaturation sites are not bonded to the metal, numerical locants are added in front of the symbol η. It may also be necessary to denote a single atom in the ligand that is directly attached to the metal; in this case, the symbol κ (kappa) is cited before the element symbol that indicate the specific position that is bonded to the metal. See ref 12a, Sections 9.2.4 and 10.2.5 for a complete discussion on the use of η and κ symbols in additive nomenclature.

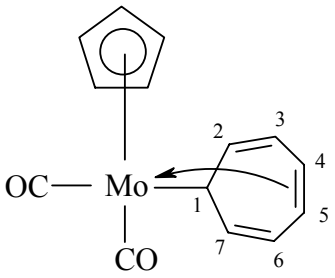
Examples:



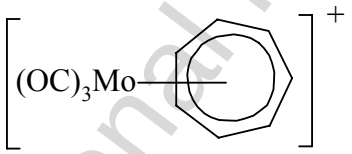
. tris(η^3-allyl)chromium



(η^4-bicyclo[2.2.1]hepta-2,5-diene)tricarbonyliron



dicarbonyl[(4,5-η,κC^1)-cyclohepta-2,4,6-dien-1-yl](η^5-cyclopentadienyl)molybdenum

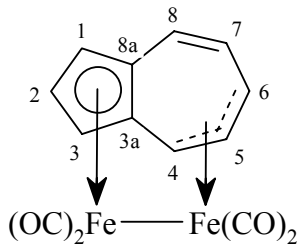


tricarbonyl(η^7-cycloheptatrienylium)molybdenum(1+)

P-69.2.4 Bridging organometallic groups with multicenter bonding to carbon atoms.

The prefix 'μ'(see I-10.8.2, ref 2) is added to the name of organometallic groups to indicate bridging between two metal atoms. Locants for the 'η' positions are separated by the colon and direct bonding between metal atoms is indicated as described in I-10.8.3.1.

Example:

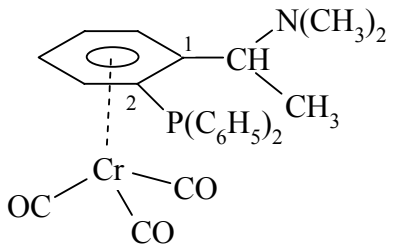


[μ-(1,2,3,3a,8a-η:4,5,6-η)-azulene]-pentacarbonyldiiron (*Fe–Fe*)

P-69.2.4 Organometallic compoloupnc with unsaturated molecules and substituent groups

Organic molecules used as ligands are named substitutively in accordance with principles, rules and conventions of substitutive nomenclature and cited in the name of the organometallic compound with the appropriate hapto symbols. This method is preferred to that consisting of using prefixes only to denote characteristic groups in the organic part of the organometallic compound.

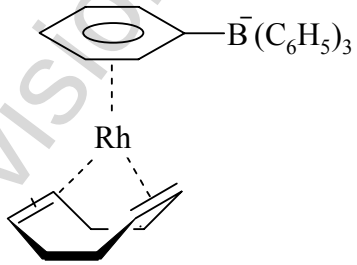
Example:



tricarbonyl{1-[2-(diphenylphosphanyl)-η^6-phenyl]-*N*,*N*-dimethylethanamine}chromium
tricarbonyl{[1-[1-(dimethylamino)ethyl)]-2-(diphenylphosphanyl)-η^6-benzene}chromium
(in the second name, the benzene ring is treated as the principal group because it is the part of the ligand attached to the metal; this method as yet has not official sanction)

In zwitterionic complexes, in which a noncoordinated atom of the ligand carries a charge which is offset by the opposite charge at the metal atom, the charge of the ligand is indicated by the appropriate ligand name ending, while the charge of the central atom is not indicated.

Example:

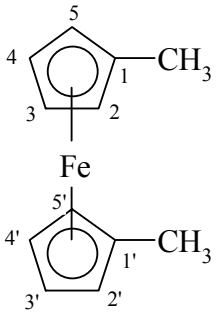


(η^4-cycloocta-1,5-diene)[(η^6-phenyl)triphenylboranuide]rhodium
(η^4-cycloocta-1,5-diene)[(triphenylboranuidyl)-η^6-phenyl]rhodium

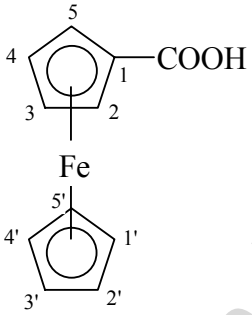
P-69.2.5 "Ocenes"

"Ocenes" are bis(η^5-cyclopentadienyl) complexes of certain metals. The names ferrocene, ruthenocene, osmocene, nickelocene, chromocene, cobaltocene and vanadocene are names for compounds corresponding to 'bis(η^5-cyclopentadienyl)metal', where the metal atom is Fe, Ru, Os, Ni, Cr, Co, and V. These names are substituted in accordance with the principles, rules and conventions of substitutive nomenclature, using suffixes or prefixes to denote characteristic groups.

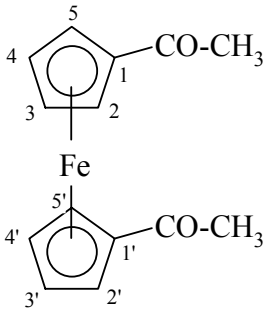
Examples:



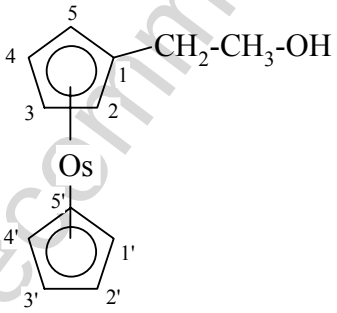
1,1′-dimethylferrocene



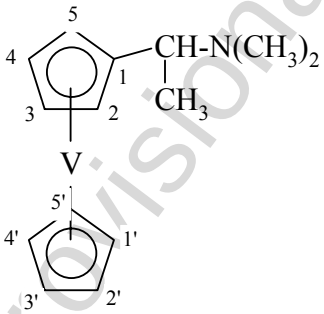
ferrocenecarboxylic acid
carboxyferrocene



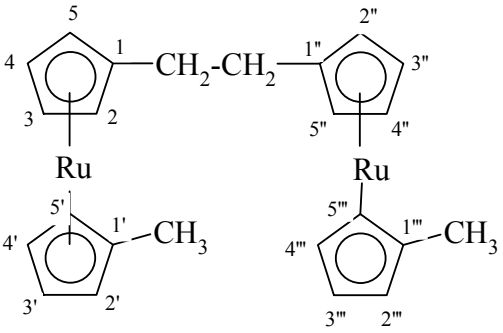
1,1′-(ferrocene-1,1′-diyl)di(ethan-1-one)
1,1′-diacetylferrocene



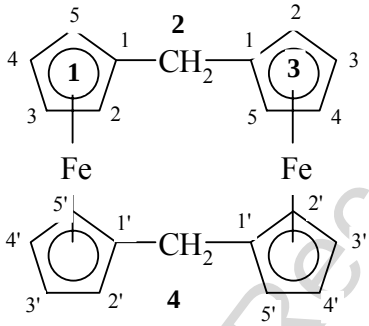
2-(osmocen-1-yl)ethanol
osmocene-2-ethanol



N,*N*-dimethyl(vanadocen-1-yl)ethan-1-amine
1-[1-(dimethylamino)ethyl]vanadocene



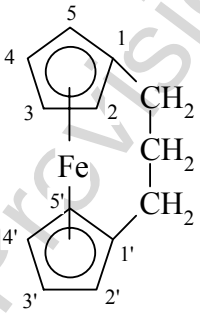
1,1″-(ethane-1,2-diyl)bis(1′-methylruthenocene)



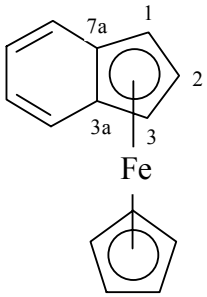
1(1,1′),3(1,1′)-diferocenacylotetraphane

Bridging and fusion principles may also be useful in naming ocene compounds.

Examples:



1,1′-propanoferrocene
1(1,1′)-ferrocenacyclotetraphane

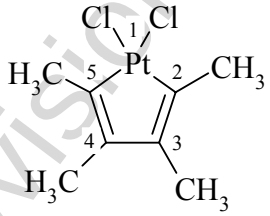


benzoferrocene
(η^5-cyclopentadienyl)[(1,2,3,3a,7a)-η^5-indenyl]iron

P-69.2.6 Metallacycles

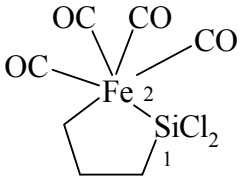
Metallacycles are organic heterocycles in which one or more heteroatoms is (are) metal atoms other than the metals normally included in the nomenclature systems for heteromonocycles (see P-22.2). They are named by extending the Hantzsch-Widman system to include the metallic elements other than those in Groups 13-16, but with a '0' standard valence and the stems 'ine' and 'inane' for unsaturated and saturated six-membered heterocycles, respectively; or by selecting a parent hydrocarbon ring or ring system and replacing one or more carbon atoms by a metal atom from Groups 2-12 using a nondetachable skeletal replacement ('a') prefix to create the metallacyclic parent hydride. The name is adjusted to conform with the observed formula by substitutions using detachable prefixes on the ring and appropriate ligand names to describe atoms or groups attached to the metal atom.

Examples

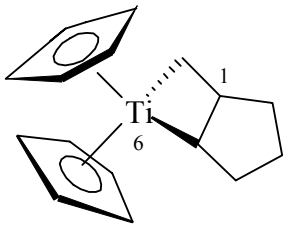


1,1-dichloro-2,3,4,5-tetramethylplatinole Hantzsch-Widman name)
1,1-dichloro-2,3,4,5-tetramethyl-1-platinacyclohexa-2,4-diene (skeletal replacement name)

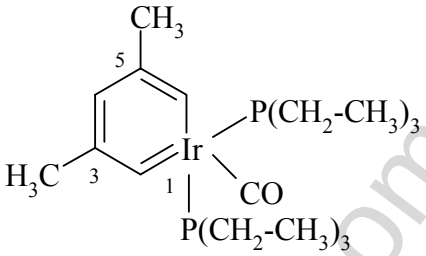
:



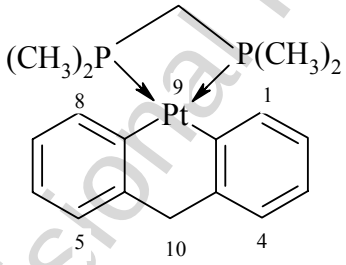
2,2,2,2-tetracarbonyl-1,1-dichloro-1,2-silaferrole (Hantzsch-Widman name)
2,2,2,2-tetracarbonyl-1,1-dichloro-1-sila-2-ferracyclopentane



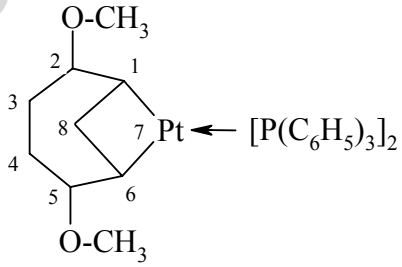
6,6-(η^5-cyclopentadienyl)-6-titanabicyclo[3.2.0]heptane



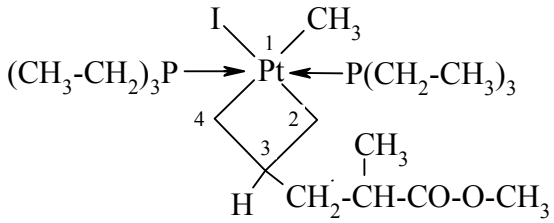
1-carbonyl-3,5-dimethyl-bis(triethylphosphane)iridin (Hantzsch-Widman name)
1-carbonyl-3,5-dimethyl-bis(triethylphosphane)-1-iridabenzene



9,9-[methylenebis(dimethylphosphane)-*P*,*P'*]-10*H*-9-platinaanthracene



2,5-dimethoxy-7,7-bis(triphenylphosphane-*P*)-7-platinabicyclo[4.1.1]octane



methyl 3-[1-iodo-1-methyl-1,1-bis(triethylphosphane-*P*)platinetan-3-yl]-2-methylpropanoate
(Hantzsch-Widman name)
methyl 3-[1-iodo-1-methyl-1,1-bis(triethylphosphane-*P*)-1-platinacyclobutyl]-2-methylpropanoate

P-69.3 Order of seniority for organometallic compounds

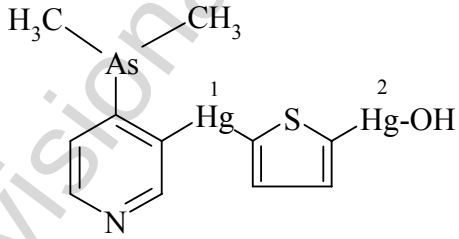
When two different metals are present in an organometallic compound, one must be chosen as the basis of the name. Metals are classifed into:

(1) metals of Groups 1 through 12; and

(2) metals (semimetals) of Groups 13 through 16.

P-69.4.1 Compounds having two identical or different metal atoms belonging to the first class are named additively using the methodology described in Section IR-9.2.5 of ref 12a, and the order of seniority of the Element Sequence Table beginning at Zn, i.e. Zn > Cd > Hg >.....Li > Na > K > Rb > Cs > Fr (see Table IV, ref. 11)

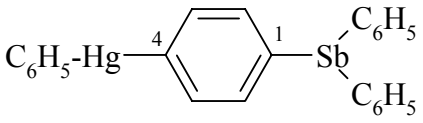
Example:



1-[4-(dimethylarsanyl)pyridin-3-yl]-2-hydroxido-μ-thiophene-2,5-diyl-dimercury

P-69.4.2 Compounds having one metal atom of class (1) and another atom of class (2) are named additively using the metal atom of class (1) as central atom, as in P-69.6.1; the other metal atom is named as a substituent group in substitutive nomenclature or as a neutral ligand.

Example:



[(4-diphenylstibanyl)phenyl]phenylmercury (PIN)

P-69.4.3 For organometallic compounds having two metal atoms belonging to class (2), substitutive nomenclature is used, as described in Section P-68. The order of priority to select the parent hydride is described in Section P-41: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > S > Se > Te > C.

Example:

$(C_6H_5)_2Bi\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}Pb(C_2H_5)_3$

diphenyl[3-(triethylplumbyl)propyl]bismuthane (PIN)

$H_2Bi\text{-}GeH_3$

germylbismuthane

$Pb(SnH_3)_4$

plumbanetetrayltetrakisstannane