

# **ACD/Labs ChemSketch (Version 8.0)**

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**Technical Note**

***ACD/Labs Principles for Representing  
Organometallic Structures***

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# ACD/Labs Principles for Representing Organometallic Structures

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## Basic Principle

The structure must be drawn in a way that correctly represents a composition, atom-atom connectivity, including the order of bonds, so that this drawing will lead to the correct total charge and molecular formula.

### 1. Representation of "Localized" Bonds

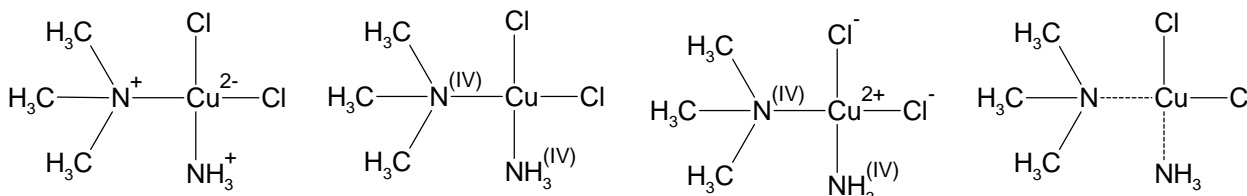
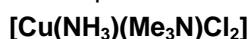
As soon as ACD/ChemSketch and most other Chemical Drawing programs use automatic calculation of atomic characteristics, care must be taken to keep the overall molecular properties correct.

The utilization of "normal" single, double, and triple bonds itself without changes (manual or automatic) of other atom properties, leads in many cases to an incorrect overall charge and/or molecular formula.

There could be at least four ways to correctly represent organometallic structures:

1. **Common bonds and additional charges.**
2. **Common bonds and nonstandard valences.** Valences may be defined implicitly or explicitly.
3. **Common bonds, nonstandard valence and charges.** (CAS uses this way in some published databases)
4. **Coordination bonds** (or zero order bonds).

The following four examples illustrate these concepts for the neutral structure



(The valence of copper is not shown)

All four structures correctly describe connectivity, net charge, and molecular formula.

Molecular Formula = C<sub>3</sub>H<sub>12</sub>Cl<sub>2</sub>CuN<sub>2</sub>

Formula Weight = 210.59278

Nonstandard valences are not shown in most cases but they must be changed otherwise the number of hydrogens and/or net charge will be incorrect. An alternative way requires the possibility to define the number of hydrogens directly or to not affect the number of hydrogens and/or charges by the attachment of additional bond.

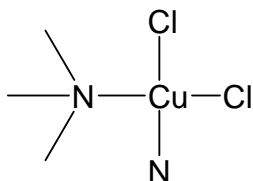
ACD/Name supports the 1<sup>st</sup> and 4<sup>th</sup> methods—charges and/or coordination bonds. Other representations are refused or analyzed as drawn according to the 1<sup>st</sup> (charges) method. ACD/Labs plans to expand the naming of coordination structures to support nonstandard valence presentations.

Only ACD/ChemSketch supports coordination bonds, hence a drawing in other drawing programs needs to use "valence" and/or "charges" methods for representation. Coordination bonds in ACD/ChemSketch can be drawn in four ways that allow you to create drawings in different ways as you prefer.

If the desired structure is drawn using normal bonds without any care about charges and the number of hydrogens, the result may be incorrect. This primarily affects coordination bonds to neutral ligands like ammonia or substituted amines

## Drawing in MDL ISIS Draw

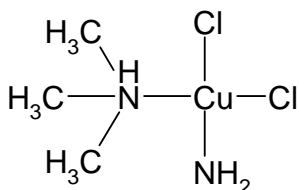
First of all you need to switch on the display of hydrogens. For example, you can draw the following structure



This structure has correct values:

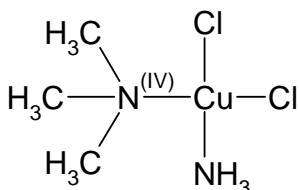
Molecular Weight = 210.59, Molecular Formula =  $C_3H_{12}Cl_2CuN_2$

But if we switch on the display of hydrogens, we will see that the positions of hydrogens are incorrect. Note that uncharged nitrogen with "auto valence" is treated by ISIS as V-valent. The structure is drawn as having V and III valent nitrogens.



The same situation occurs with phosphorus containing ligands.

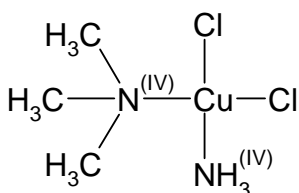
To correct the structure, the user needs to change valences or charges. The correction of valence can lead to a situation where a NH<sub>3</sub> group may be entered as a label only and the structure will look correct:



Note that even considering that the screen representation is correct, the structure has incorrect calculated values!

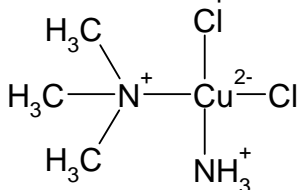
Molecular Weight = **209.59**, Molecular Formula =  $C_3H_{11}Cl_2CuN_2$

The correct structure needs to be specified with a valence of IV for the nitrogen.



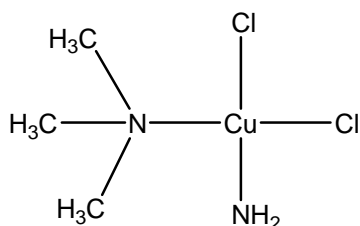
Molecular Weight = 210.59, Molecular Formula =  $C_3H_{12}Cl_2CuN_2$

Another correct representation can be achieved with charges:



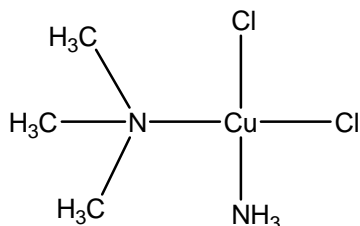
## CambridgeSoft ChemDraw

The common approach is to not show hydrogens



Molecular Weight = 209.59, Molecular Formula = C<sub>3</sub>H<sub>11</sub>Cl<sub>2</sub>CuN<sub>2</sub>

You need to enter the atom labels with hydrogens to achieve the correct number of hydrogens. Such labels will be treated as incorrect but the structure will have correct values.



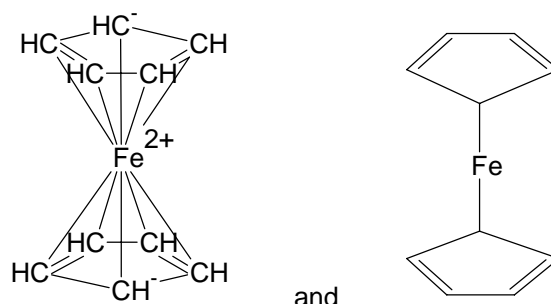
Molecular Weight = 210.59, Molecular Formula = C<sub>3</sub>H<sub>12</sub>Cl<sub>2</sub>CuN<sub>2</sub>

The display of "charge" may also be used in ChemDraw to represent coordination structures. Thus special care must be taken to represent coordination structures correctly in drawing programs.

## 2. Representation of Delocalized Bonds

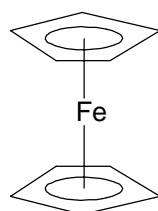
The representation of delocalized bonds is a far less well-defined area. Such structures need special procedures to define the correct bonding of the components.

Most often ferrocene-like structures are drawn in the drawing programs in the following way:



For example, some CAS databases use the first representation.

Other representations may include a radical at the cyclopentadienyl ligand. On the other hand, chemists use the following presentation:

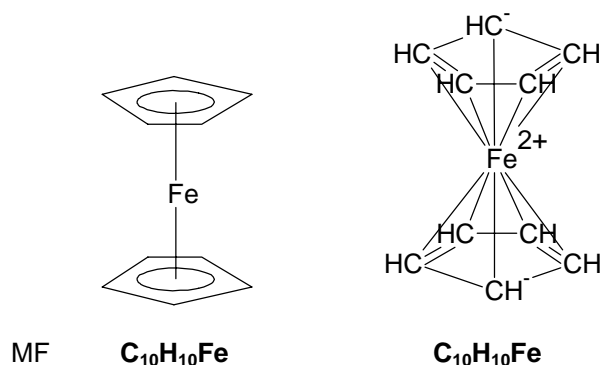


Different drawing programs use their own styles to draw such structures and such drawings cannot be exchanged between different drawing programs as chemically significant objects, except for structures that use charges and/or nonstandard valence presentations.

## ACD/ChemSketch

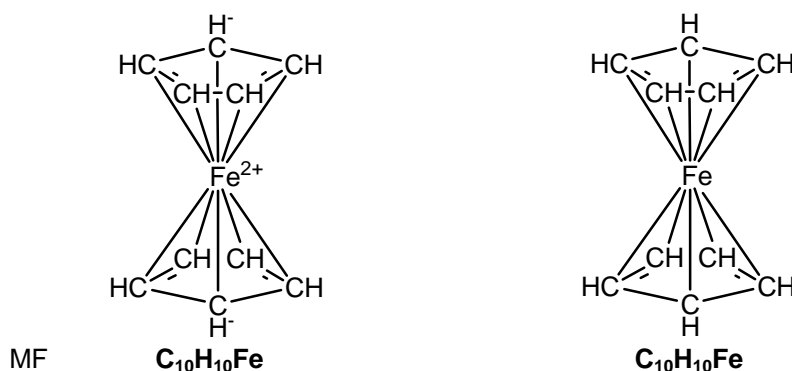
ACD/ChemSketch supports the delocalized presentation of ferrocenes and related structures. Localized presentation is also possible if the valence of the carbon centers is set to five.

For example:

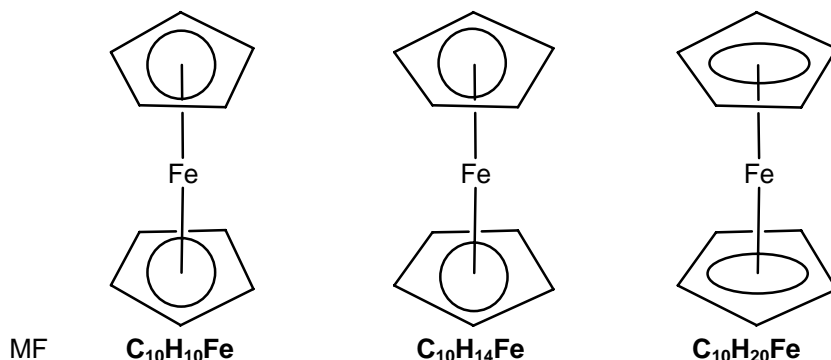


**Note** ACD/ChemSketch allows many bonds to any atom (with a warning about valence violation). At present other ACD/Labs programs do not support more than six bonds to any atom. This will be addressed in future versions.

## ChemDraw

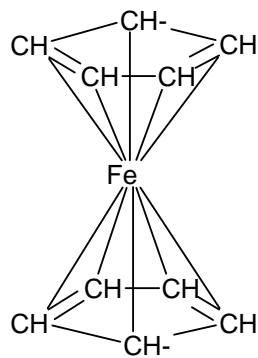


ChemDraw allows the more common presentation using multicenter attachments. The circle positioned in the five-membered ring is automatically treated as a delocalized unsaturated system. But care must be taken about the position of atoms in relation to the circle. On the other hand, an ellipse cannot be used since it is not treated as a delocalized center.



Thus almost equivalent drawings may be treated by the program in different ways as shown by the calculated molecular formulae.

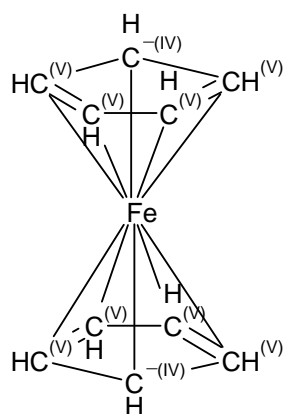
## ISIS Draw



MF

**C<sub>10</sub>Fe**

While the structure looks correct, the MF is incorrect!



MF

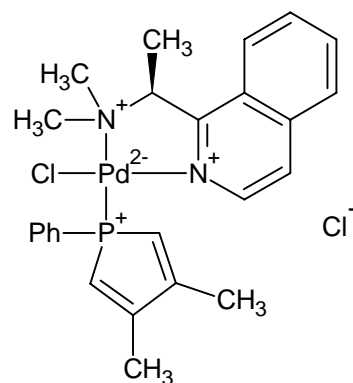
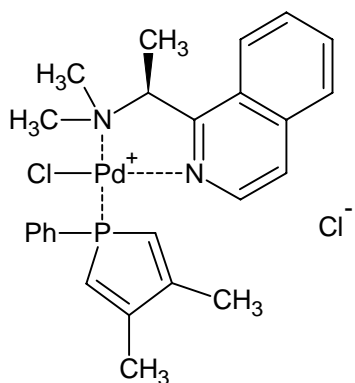
**C<sub>10</sub>H<sub>10</sub>Fe**

**Note** To keep the correct MF, some carbon atoms are IV and some are V-valent!

ISIS/Draw does not support the drawing of delocalized structures.

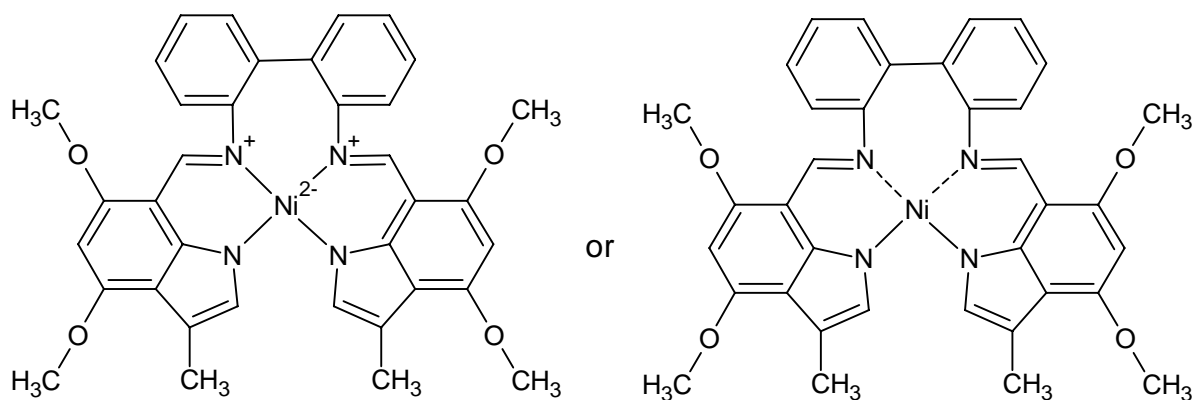
### 3. Examples of Coordination Structures Drawn in ACD/ChemSketch

Several examples showing the representation of coordination structures and the names generated by ACD/Name are given below.

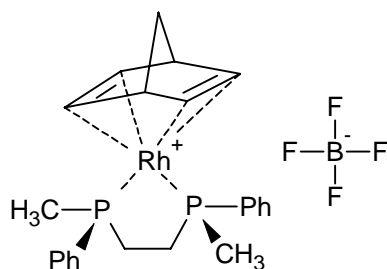


or

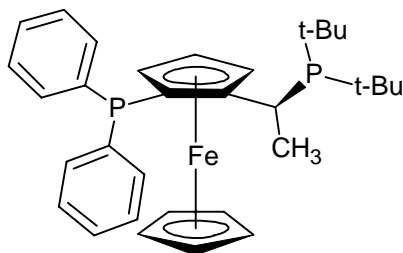
**chloro(3,4-dimethyl-1-phenyl-1*H*-phosphole)[(1*S*)-1-(isoquinolin-1-yl-κ*M*)-*N,N*-dimethylethanamine-κ*N*]palladium(1+) chloride**



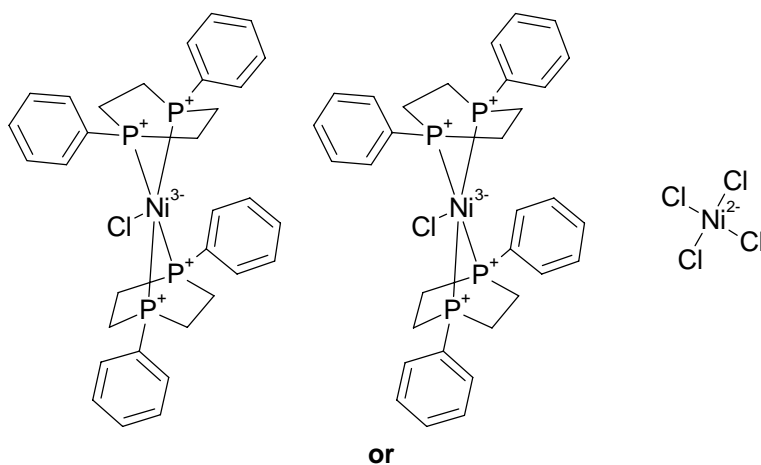
**[*N,N'*-bis[(4,6-dimethoxy-3-methyl-1*H*-indol-7-yl- $\kappa N$ )methylene]biphenyl-2,2'-diaminato(2-)- $\kappa N,\kappa N$ ]nickel**

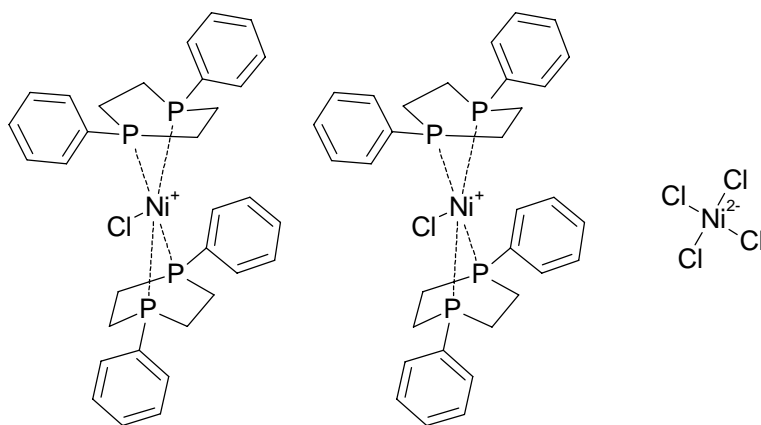


**[(2,3,5,6- $\eta$ )-bicyclo[2.2.1]hepta-2,5-diene]{ethane-1,2-diylbis[methyl(phenyl)phosphine- $\kappa P$ ]rhodium(1+) tetrafluoroborate**



**1-[(1*S*)-1-(di-*tert*-butylphosphino)ethyl]-2-(diphenylphosphino)ferrocene**





**bis[chloro[bis(1,4-diphenyl-1,4-diphosphinane- $\kappa P^1, \kappa P^4$ )]nickel(1+)] tetrachloronickelate(2-)**