

SHORT INTRODUCTION TO NOMENCLATURE OF COORDINATION COMPOUNDS

The purpose of having rules for nomenclature is simply to be able to make oneself understood while not being around to tell and make sketches. The naming rules give instructions of how to communicate unequivocally about the composition and geometry of chemical compounds using letters, numbers and a few other symbols.

1 The components

A The Central atom, which normally is a metal ion with positive charge, is surrounded by a number of ligands, which are said to be coordinated to the central atom. The bond may be called a dative bond, an expression suggesting that a lone-pair on the ligand is donated to the metal ion giving a partially covalent bond. Normally there is of course an electrostatic contribution from the attraction between the negatively polarised (or negatively charged) ligand and the positive metal ion.

B The word "coordination compound" means a compound containing a charged or non-charged central atom and a number of attached ligands. Chemical compounds do not have a net charge, so if the central atom plus the ligands have a net positive or negative charge, the coordination compound must have a counter ion. The name of the category "central atom plus ligands with a net charge" should therefore be a coordination ion. Some times you meet the expression "the complex ion" (complex means made up of several parts). Most often the word coordination compound is used for a central atom plus its ligands irrespective of the net charge and for salts composed of a coordination ion plus an appropriate number of counter ions.

2 FORMULA

A A coordination compound is given a formula, which contains the components in it with their atomic symbols and ligand formula (in many cases as an abbreviation) within square brackets and the net charge (if it is different from 0) outside the square brackets. The central atom is written first with the different ligands in a certain series:

ex. 1. The coordination compound consisting of 6 fluoride ions coordinated to a aluminium(III) ion has the formula $[\text{AlF}_6]^{3-}$

ex. 2. The coordination compound consisting of 6 water molecules coordinated to a aluminium(III) ion has the formula $[\text{Al}(\text{H}_2\text{O})_6]^{3+}$

B If different ligands are present in the same coordination compound these are given in a series, where negatively charged ligands are first, the non charged ones next, and finally positively charged ligands.

ex. 3. The coordination compound consisting of 4 fluoride ions and 2 water molecules coordinated to a aluminium(III) ion has the formula $[\text{AlF}_4(\text{H}_2\text{O})_2]^-$

C If different ligands of same charge type (i.e. negative, non charged or positive) are present in the same coordination compound they are given in alphabetic order within the same charge group.

ex. 4. The coordination compound consisting of 4 ammonia molecules and 2 water molecules coordinated to a chromium(III) ion has the formula $[\text{Cr}(\text{NH}_3)_4(\text{H}_2\text{O})_2]^{3+}$

ex. 5. The coordination compound consisting of 4 ammonia molecules and 2 fluoride ions coordinated to a chromium(III) ion has the formula $[\text{CrF}_2(\text{NH}_3)_4]^+$

ex. 6. The coordination compound consisting of 4 ammonia molecules and 1 fluoride ion and 1 chloride ion coordinated to a chromium(III) ion has the formula $[\text{CrClF}(\text{NH}_3)_4]^+$

ex. 7. The coordination compound consisting of 3 ammonia molecules and 1 water molecule,

1 fluoride ion and 1 chloride ion coordinated to a chromium(III) ion has the formula $[\text{CrClF}(\text{NH}_3)_3(\text{H}_2\text{O})]^+$. This example also illustrates, that some times a ligand is given in brackets even if there is only one of the kind; it makes it easier to read the formula. To write $[\text{Cr}(\text{Cl})(\text{F})(\text{NH}_3)_3(\text{H}_2\text{O})]^+$ is perhaps a little over-kill, but on the other hand very easy to understand.

D The spatial arrangement of ligands relative to each other can also be described in a formula: Thus it is simple to put a *cis* or a *trans* (or a *fac* or a *mer*) – in *italics* - together with a hyphen in front of the square brackets. Of course, this requires a knowledge of the geometric isomerism. Optical isomers are given (followed by a hyphen in front of the square brackets) with a Δ or a Λ

ex. 5. continued The coordination compound consisting of 4 ammonia molecules and 2 fluoride ions coordinated to a chromium(III) ion could either be *cis*- $[\text{CrF}_2(\text{NH}_3)_4]^+$ if the two fluoride ions are close to each other, or *trans*- $[\text{CrF}_2(\text{NH}_3)_4]^+$, if the two fluoride ions are opposite to each other in the octahedron.

ex. 8 The coordination compound consisting of 3 ammonia molecules and 3 fluoride ions coordinated to a chromium(III) ion with the formula $[\text{CrF}_3(\text{NH}_3)_3]$ could either be *fac*- $[\text{CrF}_3(\text{NH}_3)_3]$, if the three fluoride ions are close to each other in the octahedron or be *mer*- $[\text{CrF}_3(\text{NH}_3)_3]$, if two of the three fluoride ions are opposite to each other in the octahedron

NAMES

A If the compound consists of one or more cations and one or more anions, the cation (-s with numbers as prefixes) are mentioned first, anion (-s with numbers as prefixes) in the end. This follows the normal rules for naming of salts.

B The ligands are mentioned before the central atom.

C Negatively charged ligands are normally given the name of its parent element (or the name of the complex ion) followed by an o.

D Neutral ligands is given its own name (except aqua for water, ammine for ammonia, nitrosyl for nitrogenmonoxid and carbonyl for carbonmonoxid – see below)

E The number of a given ligand is given by a number-prefix. Mono- di-, tri-, tetra-, penta-, hexa-, unless the ligand name is particularly long or complicated or itself starts with a number-prefix. In such cases the terms bis-, tris-, tetrakis-, pentakis- ... are used.

F Different ligands in the same coordination compound are given in strictly alphabetic order of the ligands (number-prefixes has no influence on that)

G Bridging ligands (between two central atoms) is given the prefix μ

H Ambidentate ligands (composed of more atoms - ligands, which can bind in more than one way especially with the lone-pair on different atoms) may be designated by the way it actually binds (if it is known). The nitrite ion may bind through O and is then called nitrite, or through its N when it is called nitro. The thiocyanate ion coordinating through S is named thiocyanato, whereas the N-bound thiocyanate is called isothiocyanato.

I The central atom is normally characterised by its oxidation number by a bracketed roman number after the name of the central atom. This is not necessary in the cases where the central atom only appears in one oxidation state (but it is not forbidden to give the oxidation state).

J If the coordination compound is a cation or non-charged the cations name is used without any ending. In the first case the anions name in the salt may be given. If the coordination compound itself is an anion the ending -ate is added to the name of the central atom (including its oxidation state)

Ex. 8 $[\text{Cr}(\text{NH}_3)_6]^{3+}$ is called hexaamminechromium(III) (rule B, D, E, J and I)

Ex. 1 $[\text{AlF}_6]^{3-}$ is called hexafluoroaluminate (rule B, C, E, I and J)

- Ex. 2 $[\text{Al}(\text{H}_2\text{O})_6]^{3+}$ is called hexaaquaaluminium (rule B, D, E, I and J)
 Ex. 3 $[\text{AlF}_4(\text{H}_2\text{O})_2]^-$ is called diaquatetrafluoroaluminate (rule B, C, D, E, F, and I)
 Ex. 9 $[\text{Mg}(\text{H}_2\text{O})_6](\text{SO}_4)$ is called hexaaquamagnesium sulphate (rule A, B, D, E, and J). The compound is also found under the name magnesium sulphate, unless it should explicitly be distinguished from the water free MgSO_4 , which is not a coordination compound, but a simple salt only existing as such in the solid state.
 More examples are found in Chang's General Chemistry (or other undergraduate texts).

Further here are some special ligand names for

water	aqua
ammonia	ammine
(methyl)amin	amine
nitrogenmonoxid (NO)	nitrosyl
carbonmonoxid (CO)	carbonyl
dinitrogen (N_2)	dinitrogen
dioxygen (O_2)	dioxygen

To practise:

Write a correct formula for the following compounds and sketch the spatial arrangement

- cis*-Tetraaquadichlorochromium(III) chloride
 Potassium pentachloronitrosmiate(IV)
mer-Trihydridotris(triphenylphosphine)ruthenium(III)
 Pentaamminchlorocobalt(III) nitrate
 Potassium trisoxalatocobaltate(III)
 Bis(1,2-ethanediamine)diiodocobalt(III) perchlorate
 Dichlorobis(1,2-ethanediamine)cobalt(III) tetrafluoroborate
 Pentaamminedinitrogenruthenium(II) chloride
 Sodiumpentacyanonitrosylferrate(II) dihydrate
 Pentaamminecobalt(III)- μ -cyanopentacyanocobaltate(III)

Give a name to the following compounds

- $[\text{PtCl}_2(\text{NH}_3)_2]$
 $[\text{RhCl}(\text{NH}_3)_5]\text{Cl}_2$
 $[\text{Co}(\text{NH}_3)_6]\text{SO}_4$
 $[\text{Co}(\text{NH}_3)_4(\text{H}_2\text{O})_2](\text{BF}_4)_3$
 $\text{Na}_3[\text{Fe}(\text{CN})_6] \cdot 2\text{H}_2\text{O}$,
 $[\text{Ni}(\text{CO})_4]$,
 $[\text{Co}(\text{CH}_3\text{COO})\text{BrCl}(\text{NH}_3)_2]$,
 $[\text{Pt}(\text{py})_4] [\text{PtCl}_4]$,
 $\text{Na}_2[\text{PdCl}_6]$,
 $(\text{NEt}_4)_3[\text{AlF}_6]$,
 $[\text{Pt}(\text{acac})_2\text{ClNH}_3]\text{Cl}$

acac is the abbreviation for acetylacetonato which is the deprotonated acetylacetonone
 py is the abbreviation for pyridine
 en is the abbreviation for 1,2-ethanediamine
 Et is ethyl in for example tetraethylammonium, NEt_4^+
 acetate is often abbreviated as Ac