IUPAC Nomenclature of Coordination Compounds

Coordination compounds adhere to a system established by the International Union of Pure and Applied Chemistry (IUPAC) for formulation and nomenclature. This system is crucial for accurately expressing systematic names and formulas, especially in cases involving isomers.

Rule for Writing Formulae of Mononuclear Coordination Entities

Obtaining information about the constitution of a compound becomes significantly more accessible when we possess its formula. Mononuclear entities, which consist of a single central atom, provide a clear framework for formula writing. To construct the formula, specific rules are followed:

(i) The central atom is prioritized and listed first.

(ii) Subsequently, ligands are arranged alphabetically, disregarding their charges, to ensure consistency in formula representation.

(iii) When dealing with abbreviated ligands, particularly those that are polydentate, the position of the ligand in alphabetical order is determined by the first letter of its abbreviation.

(iv) The entire coordination entity, whether charged or neutral, is enclosed within square brackets. Polyatomic ligands, along with their abbreviations, are enclosed within parentheses.

(v) There should be no space between the names of ligands and the central atom/ion.

(vi) When writing the formula of a charged coordination entity without including the counter ion, the charge is denoted outside the square brackets as a right superscript, with the numerical value placed before the sign. For example, $[Co(CN)_6]^{3-}$, $[Cr(H_2O)_6]^{3+}$.

(vii) The charge on the cation and anion is balanced by the appropriate counter ion.

Rule for Naming of Mononuclear Coordination Compounds

By employing the principles of additive nomenclature, it is essential to identify the groups surrounding the central atom within coordination compounds. These groups are listed as prefixes preceding the name of the central atom.

The following rules govern the naming of coordination compounds:

(i) The positive portion of complex compounds is named first, followed by the negative portion.

(ii) Ligands are alphabetically named before the central atom (in reverse order when writing the formula).

(iii) Numerical prefixes such as mono-, di-, tri-, tetra-, etc., are utilized to indicate the number of ligands. For complex ligands, including a numerical prefix, bis-, tris-, tetrakis- are applied. For instance, $[NiCl_2(en)_2]SO_4$ is named as dichloridobis (ethylene diamine) nickel (II)sulphate.

(iv) Anionic ligands' names conclude with 'o', while cationic ligands end with 'ium'. Neutral ligands retain regular names, with exceptions such as 'aqua' for H_2O, 'ammine' for NH_3, 'nitrosyl' for NO, and 'carbonyl' for CO, which are enclosed within parentheses.

(v) The oxidation state of the central atom/ion is denoted in Roman numerals within brackets following the name of the metal.

(vii) If the coordination compound carries a negative charge, the central metal's name is suffixed with 'ate'; otherwise, this suffix is not added. For instance, in $[Fe (CN)_6]^{4-}$, the term 'ferrate' is applied to denote the negative charge associated with Fe.

(viii) Examples of anionic ligands include HS^- (mercapto), CN^- (cyano), NC^- (Isocyano), F^- (fluorido), OH^- (hydroxo), N_3^- (azido), N^{3-} (nitrido), SCN^- (thiocyanato-S), NCS^- (thiocyanato-N), ONO^- (nitrito-o), and NO_2^- (nitrito-N). Examples of cationic ligands encompass $NH_2–NH_3^+$ (hydrazinium), NO^+ (nitrosonium), and NO_2^+ (nitronium).

The rules are exemplified through the following instances:

(i) $[Pt(NH_3)_4][PtCl_4]$ - Identified as Tetraammine platinum (II) tetrachloridoplatinate (II)
(ii) $[NiCl_2\ (PPh_3)_2]$ - Described as dichloridobis(triphenylphosphine)nickel (II)
(iii) $[Mn(H_2O)_6]^{2+}$ - Known as hexaaquamanganese (II) ion
(iv) $[Ni(NH_3)_6]Cl_2$ - Identified as hexaamminenickel (II) chloride
(v) $Ni(CO)4$ - Known as tetracarbonyl nickel (0)