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Structural Coordination Compound Nomenclature. Designation of Coordination Sites for Ambidentate and Flexidentate Ligands

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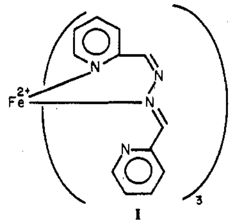
A topologically exact notation is proposed for coordination compounds which contain ambidentate and flexidentate ligands. This notation uses the Greek letter kappa (κ) preceding the italic atomic symbol locant after the portion of the ligand name to which it applies. Minor changes are proposed in the *hapto* notation and with these changes the *hapto* and kappa systems are wed to provide an unambiguous and broadly applicable nomenclature notation for coordination and organometallic compounds.

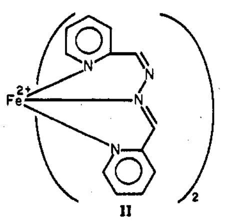
Introduction

During the early development of inorganic and coordination chemistry, the number of known compounds was relatively small and their structures were either simple or unknown. Under those conditions, trivial and nonstructural names were adequate for it was possible to remember the names, compositions, and/or structures (when known) of the compounds of interest to the individual chemist. Due to the proliferation of synthetic inorganic chemistry, this condition no longer exists: of the 4 million chemical substances in the Chemical Abstracts Service Registry System as of mid-1977, it is estimated that about 400 000 are inorganic and coordination compounds, and it is known that the number of inorganic and coordination compounds is growing at an accelerating rate. From these observations and the knowledge that the structures of new coordination compounds are of ever-increasing complexity, it is reasonable to conclude that a structurally exact inorganic coordination nomenclature is essential.

For example, the existence of linkage isomerism among complexes of ambidentate ligands has been recognized since the time of Werner. The two classical examples are nitro–nitrito compounds of cobalt prepared by Jørgensen and the thiocyanato–isothiocyanato compounds of palladium prepared at a much later date by Basolo et al.[1] With the continuing development in the chemistry of coordination compounds has come the synthesis and study of derivatives of the more complex flexidentate ligands. The articulation of the structural variations represented by flexidentate chelation accompanied the report on the various modes of chelation of 2-pyridinecarboxyaldehyde azine.[2] Complexes of the composition Fe^{2+}:3 ligand and Fe^{2+}:2 ligand were assigned structures I and II.



I



II

Flexidentate chelation involves variation in the points of attachment of the ligand and the metal ion and/or variations in the topology of chelation. Many hundreds of metal compounds have been prepared from ambidentate and flexidentate ligands in one or more isomeric forms. Ambidentate and flexidentate ligands may be as simple as the nitrito or thiocyanato ligands, or more complex, for example, as *N*-[2-(2-pyridyl)-4-thiazolyl]-2-pyridinamine. Of even greater complexity is the biologically important macrocyclic compound, the corrin nucleotide base 2,7,18-tris(carbamoylmethyl)-N^{17}-(2-hydroxypropyl)-1,2,5,7,12,12,15,17-octamethyl-3,8,13,17-corrintetrapropionamide dihydrogen phosphate (ester) 3′-ester with 5,6-dimethyl-1-α-D-ribofuranosyl-1*H*-benzimidazole, the ligand on cobalt(III) in vitamin B_{12}.

Fernelius[3] et al. first proposed a structurally specific notation for ambidentate and flexidentate ligand complexes which was incorporated into the 1957 IUPAC rules of nomenclature for inorganic chemistry.[4] Paragraph 7.33 of these rules codifies the established practice of using nitro for nitrogen-attached NO_2^- and nitrito for oxygen-attached NO_2^- and thiocyanato and isothiocyanato for the sulfur- and nitrogen-attached SCN^-, respectively. This paragraph also establishes the international sanction for the use of the italic atomic symbol of the ligand donor atom (ligating atom) at the end of the ligand name. The second edition of the IUPAC rules of nomenclature for inorganic chemistry[5] elaborates on the use of the italicized atomic symbol (ligand locant) by providing for the use of superscript locants and primes to distinguish between the same type of donor atom and defines a set of priorities for giving the ligand locant at the end of a more complicated ligand name. These priorities are based on a ligating atom priority, organic nomenclature and organic functional priority, oxidation state, chelating ring size, and ligand symmetry.

A modification of the IUPAC ligand locant approach is used in Chemical Abstracts Substance Index names in the 9th Collective Period (Volumes 76–85, 1972–1976)[6] to denote ligand attachments in coordination compounds. The ligand locants are cited in alphabetical order of the atomic symbol at the end of the ligand name with primes or numerical and atomic symbol indexes which relate directly to the parent portion of the ligand name, e.g., that portion of the ligand name expressing the basic chain, ring, and/or principal function.

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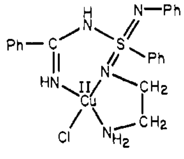
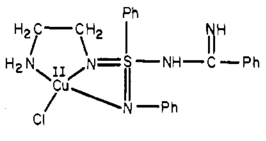
Structures I and II provide useful illustrations of the CAS procedures. In the ligand the nitrogen atoms are labeled *N*, *N*′, *N*″, and *N*‴, beginning at the nitrogen of one pyridine ring and proceeding to the other extremity of the ligand. Thus, I is tris(2-pyridinecarboxaldehyde azine-*N*,*N*″)iron(II), and II is bis(2-pyridinecarboxaldehyde azine-*N*,*N*′,*N*‴)iron(II).

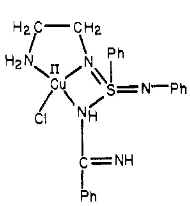
Neither the IUPAC ligand locants nor the Chemical Abstracts modification has proved wholly satisfactory due to either the complexity of the priorities for the application of the ligand locants or the ambiguity of the indexes when more complicated flexidentate ligands are encountered. These difficulties arise almost exclusively from the modular nature of the substitutive organic nomenclature employed in the naming of the more extensive ligand structures. This can be illustrated by examining hypothetical structures, III, IV, and V.



III



IV



V

The name "[*N*′-[*N*-(2-aminoethyl)-*N*′,*S*-diphenylsulfonodiimidoyl]benzamide]chlorocopper(II)" is not structurally descriptive for compounds III, IV, and V without a method for denoting the ligand atoms attached to the copper atom.

In order to overcome these difficulties (complex priorities and ambiguous indexes), Lozac'h[7] and Gustafson[8] suggested that the ligand locant be given as an infix directly following the coordinated grouping in the organic name of the ligand. The names for structures III, IV, and V may then be written as follows: III, [*N*′-[*N*-(2-amino-*N*-ethyl)-*N*′,*S*-diphenylsulfonodiimidoyl-*N*]benzamidine-*N*′]chlorocopper(II); IV, [*N*′-[*N*-(2-amino-*N*-ethyl)-*N*′,*S*-diphenylsulfonodiimidoyl-*N*,*N*′]benzamidine]chlorocopper(II); V, [*N*′-[*N*-(2-amino-*N*-ethyl)-*N*′,*S*-diphenylsulfonodiimidoyl-*N*]benzamidine-*N*]chlorocopper(II). These names with locants constitute a nomenclature set which reflects the structure exactly. However, inspection of these names readily indicates that the organic nomenclature locants and the coordination ligand locants are so similar that it is not immediately obvious which is the organic locant and which is the ligand locant.

The notation developed throughout this paper is illustrated with mononuclear complexes. It should be obvious that the notation we present is extendable to polynuclear complexes.[9] We also note that specialized symbols, e.g., μ and η, have proven to be very useful in the nomenclature of coordination and organometallic chemistry. The symbol μ has been used since near the beginning of the field. It is our intention to augment these established practices with minimum modifications.

Principles of the Kappa Convention

The wish to propose an adaptation and extension of the coordination ligand locant device to provide a simpler, topologically explicit, and readily discernible notation for coordination nomenclature. The notation is defined as follows:

1. Single ligating atom attachments of a polyatomic ligand to a coordination center are indicated by the italic element symbol preceded by a Greek kappa (κ).

2. The ligand locant is placed after that portion of the ligand name to which it directly applies: that is, after that part of the ligand name which denotes the parent function, ring, chain, or radical prefix in which the ligating atom is expressed. Ligating atoms expressed in functions, chains, rings, and radical prefixes which contain other donor atoms are uniquely indicated by a superscript numeral, letter, or prime on the element symbol. These indexes denote the position of the ligating atom in the function, chain, ring, or radical prefix.

3. For polydentate ligands a superscript numeral may be given on the κ to indicate the number of identically bound ligating atoms in the flexidentate ligand.

Monodentate ambident ligands provide the simplest examples. Nitrogen-bonded NO_2^- is nitrito-κN while O-bonded NO_2^- is nitrito-κO. Similarly, N-bonded NCS is thiocyanato-κN (as in $[Co(NCS)_4{}^{2-}]$, tetrakis(thiocyanato-κN)cobaltate(II)) and S-bonded NCS, thiocyanato-κS. The names corresponding to structures I and II are tris(2-pyridinecarboxaldehyde-κN azine-$\kappa N'$)iron(II) and bis(2-pyridinecarboxaldehyde-$\kappa^2 N$ azine-κN)iron(II).[10]

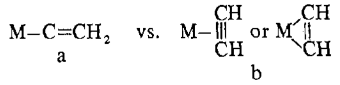
Under this system, structures III, IV, and V have the following names: III, [*N*′-[*N*-(2-amino-κN-ethyl)-*N*′,*S*-diphenylsulfonodiimidoyl-κN]benzamidine-$\kappa N'$]chlorocopper(II); IV, [*N*′-[*N*-(2-amino-κN-ethyl)-*N*′,*S*-diphenylsulfonodiimidoyl-κN,$\kappa N'$]benzamidine]chlorocopper(II); V, [*N*′-[*N*-(2-amino-κN-ethyl)-*N*′,*S*-diphenylsulfonodiimidoyl-κN]benzamidine-κN]chlorocopper(II).

This notation is capable of giving absolute definition to the points of attachment to metal ions of immensely complicated ligands as, for example, in the case of the vitamin B_{12} species, (cyano-κC)[2,7,18-tris(carbamoylmethyl)-N^{17}-(2-hydroxypropyl)-1,2,5,7,12,12,15,17-octamethyl-3,8,13,17-corrintetrapropionamide-κN^{21},κN^{22},κN^{23},κN^{24} dihydrogen phosphate (ester) 3′-ester with 5,6-dimethyl-1-α-D-ribofuranosyl-1*H*-benzimidazolato(2−)-κN^3]cobalt(III).

Relationship to the *Hapto* Convention

The *hapto* notation introduced by Professor Cotton for olefin–metal complexes has been widely adopted in the current chemical literature. Some confusion in application of the *hapto* notation has occurred because of certain subtle differences between the original exposition of the *hapto* principles[11] and that adopted by the IUPAC Commission. The IUPAC Commission states in Table III[12]: "...η signifies that two or more contiguous atoms of a group are attached to a metal..." which is nowhere stated in ref 11. Professor Cotton in the original exposition of *hapto* was careful to indicate the precise number of ligating atoms, e.g., *trihapto*, η^3; *hexahapto*, η^6, etc. This extremely important aspect of the innovation was not presented in the IUPAC version and a less exact practice was suggested in which the *hapto* symbol, without index or prefix, is used to designate "...all the multiply-bonded ligating atoms bound to a central atom." IUPAC proceeds to use locants in those instances in which all multiply bonded atoms are not bound to the central atom. We now know that many, if not the majority, of these systems are fluxional and in many specific examples giving locants that pertain to any instantaneous structure can be more misleading than simply stating the number of atoms attached to the central atom. The use of the numerical index on the *hapto* symbol provides the most economical device for providing a topologically exact name in which there may be many ligating atoms in a grouping.

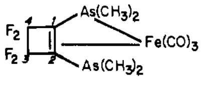
We justify the use of the two symbols, κ and η, on the basis that the difference between a single ligating atom and a ligating grouping is structurally significant and can be experimentally demonstrated, e.g.,



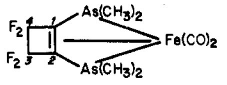
$$\underset{a}{M{-}C{=}CH_2} \quad \text{vs.} \quad \underset{b}{M{-}\overset{CH}{\underset{CH}{\|\!|}} \text{ or } M\overset{CH}{\underset{CH}{\|}}}$$

The κ and η symbols clearly distinguish between these two structures and there is no need to choose among various theoretical models concerning electron delocalization for such identification.

Because the *hapto* notation as introduced by Professor Cotton is widely accepted and provides, in a very economical way, a precise description of certain complex chemical structures, we have used his original system for *polyhapto* structures. In the examples treated here the *hapto* notation is used to indicate a structure with two or more adjacent atoms in a ligating grouping simultaneously bonded to a coordination center such that the bonding between the ligating grouping and the central atom is not assignable specifically to any single atom of the ligating group. The Greek letter eta (η) is used as the *hapto* symbol[13] and will be placed *after* the olefin or unsaturated grouping name or the name of a radical in a more complex unsaturated ligand. Placing the *hapto* symbol after the radical or unsaturated group name will collect the ligand locants consistently together at the end of the ligand name or after a ligating group name which is a prefix to the parent portion of the ligand name. When locants are used in conjunction with η, both locants and symbol are enclosed in parentheses. Thus, the name associated with structure VI is tri(carbonyl-κ*C*)[[3,3,4,4-tetrafluoro-1-cyclobutene-1,2-diyl(1,2-η)]bis[dimethylarsine]-κ*As*]iron(0) while that for structure VII is di(carbonyl-κ*C*)[[3,3,4,4-tetrafluoro-1-cyclobutene-1,2-diyl(1,2-η)]bis[dimethylarsine]-κ²*As*]iron(0).



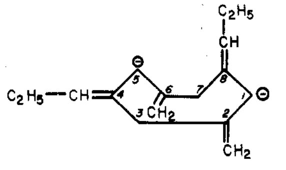
VI



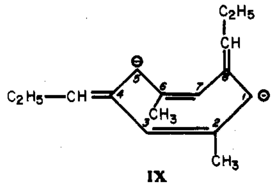
VII

Further examples will illustrate the topological exactness of this proposed notation and its compatibility with the *hapto* notation. Either certain portions of the example structures have been modified to emphasize the coordinating groups by using simpler noncoordinating substituent groups rather than those found in the reported compounds or composite examples were constructed to better test the versatility of the proposed notation. All examples are based on reported model structures and, where exact examples are used, references to the structures are given.

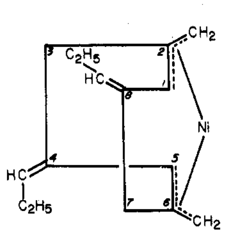
The *hapto* convention is well illustrated by the ligands given in structures VIII and IX, as they appear in complexes X and XI below. The ligand structures show the origins of the ligand names that accord with current nomenclature practice. The hypothetical carbon anion is named as a radical with a localized π-electron system.



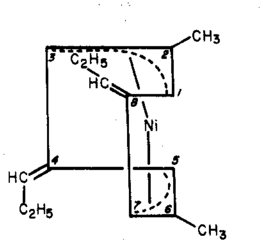
VIII



IX



X

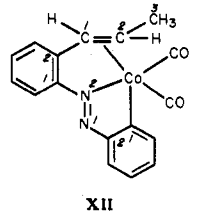


XI

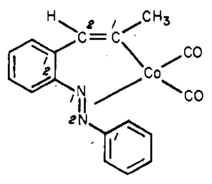
X, [2,6-di(methylene-η)-4,8-dipropylidene-1,5-cyclooctanediyl-(1,2,5,6-η)]nickel

XI, [2,6-dimethyl-4,8-dipropylidene-2,6-cyclooctadiene-1,5-diyl-(1,2,3,5,6,7-η)]nickel

The occurrence of groups in structures that simultaneously require the use of η and κ is illustrated by examples XII, XIII, and XIV. The first two are isomers in which the groups requiring the η and κ designations are interchanged.



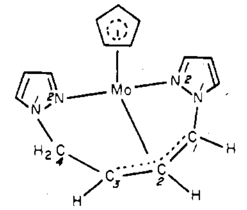
XII



XIII

XII, di(carbonyl-κ*C*)[2-[[2-[1-propenyl(1,2-η)]phenyl]azo-κ*N*²]-phenyl-κ*C*²]cobalt

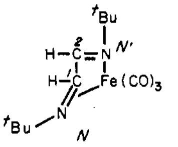
XIII, di(carbonyl-κ*C*)[1-methyl-2-[2-(phenylazo-η²)phenyl]-ethenyl-κ*C*¹]cobalt



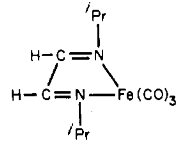
XIV

XIV, (cyclopentadienyl-η⁵)[1,4-di-1*H*-pyrazol-1-yl-κ²*N*²-2-butenyl(1,2,3-η)molybdenum

This system of notation is equally effective in those cases where π complexes are formed with functional groups containing heteroatoms, as exemplified by the structures XV and XVI. Example XVII elaborates on this category of structures by presenting a case where two different heteroatoms are involved in the delocalized group. It should be noted that the superscripts on η and κ continue to serve their roles as multiplicative indexes while, in the case of κ, the superscript affixed to the heteroatom symbol (following κ) is a locant. A subsequent X-ray determination has shown that XVIII is the correct structure for the compound tentatively assigned XVII. The two structures indicate how the notation may be applied to distinguish the *dihapto* and *trihapto* derivatives.



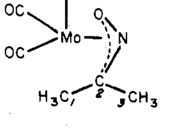
XV



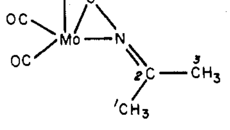
XVI

XV, tri(carbonyl-κ*C*)[*N,N′*-ethanediylidene(1-η)bis[*tert*-butylamine](*N*-η),κ*N′*]iron[14]

XVI, tri(carbonyl-κ*C*)[*N,N′*-ethanediylidenebis[isopropylamine]-κ²*N*]iron(0)[14,15]



XVII



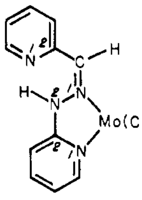
XVIII

XVII, [acetone(2-η) oximato-η²]di(carbonyl-κ*C*)(cyclopentadienyl-η⁵)molybdenum[16]

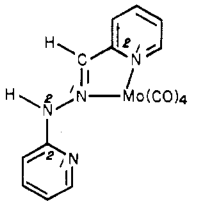
XVIII, [acetone oximato-η²]di(carbonyl-κ*C*)(cyclopentadienyl-η⁵)-molybdenum[17]

Applications Involving Complicated Polydentate Ligands

Examples XIX and XX return the focus to the points of coordination in polydentate chelates of some complexity. These cases are particularly effective at showing the placement of kappa in the name: it must appear immediately after the citation of that portion of the structure containing the ligating atoms.



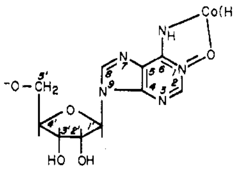
XIX



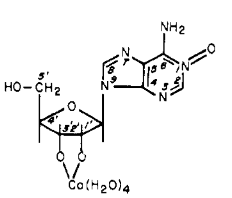
XX

XIX, tetra(carbonyl-κC)(2-pyridinecarboxaldehyde 2-pyridyl-κN-hydrazone-κN^1)molybdenum(0)[18]
XX, tetra(carbonyl-κC)(2-pyridinecarboxaldehyde-κN 2-pyridylhydrazone-κN^1)molybdenum(0)[18]

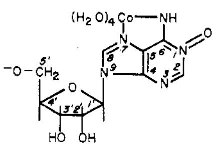
The adenosine moiety, an extreme polyfunctional ligand, is chosen in order to display the effectiveness of this system in distinguishing among a wide variety of alternative flexidentate modes of coordination (structures XXI through XXV).



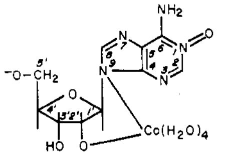
XXI



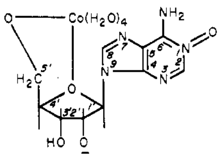
XXII



XXIII



XXIV

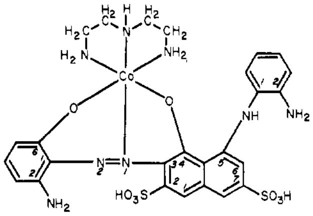


XXV

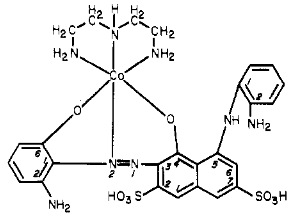
XXI, [adenosine-κN^6 1-oxidato(2−)-κO]tetraaquacobalt(II)
XXII, [adenosine-$\kappa O^{2'}$, $\kappa O^{3'}$ 1-oxidato(2−)]tetraaquacobalt(II)
XXIII, [adenosine-κN^6, κN^7 1-oxidato(2−)]tetraaquacobalt(II)
XXIV, [adenosine-κN^9, $\kappa O^{2'}$ 1-oxidato(2−)]tetraaquacobalt(II)
XXV, [adenosine-$\kappa O^{4'}$, $\kappa O^{5'}$ 1-oxidato(2−)]tetraaquacobalt(II)

The problem of designating the exact manner of binding in flexidentate ligands is very common among metal chelates of dyes. For that reason, examples XXVI through XXIX are presented below.

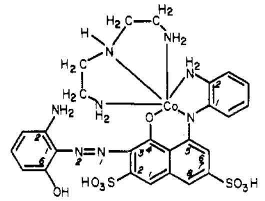
As has been the case with the *hapto* notation, the kappa principles can be successfully employed in abbreviations and formulas for coordination compounds with ligands of intermediate complexity. A few examples from the compounds listed above will serve to illustrate: I, $[Fe[(2\text{-}C_5H_4NCH)_2\text{-}\kappa N\text{-}N_2\text{-}\kappa N']_3]^{2+}$; II, $[Fe[(2\text{-}C_5H_4NCH)_2\text{-}\kappa^2 N\text{-}N_2\text{-}\kappa N]_2]^{2+}$ or $[Fe[(2\text{-}C_5H_4NCH)_2\text{-}\kappa N,\kappa N'\text{-}N_2\text{-}\kappa N]_2]^{2+}$; XII, $[Co(CO\text{-}\kappa C)_2[2\text{-}[[2\text{-}[C_3H_5(1,2\text{-}\eta)]C_6H_4]N_2\text{-}\kappa N^2]C_6H_4\text{-}\kappa C^1]]$; XIII, $[Co(CO\text{-}\kappa C)_2[1\text{-}CH_3\text{-}2\text{-}[2\text{-}(C_6H_5N_2\text{-}\eta^2)C_6H_4]C_2H\text{-}\kappa C^1]]$; XXI, $[Co(Ado\text{-}\kappa N^6\text{-}1\text{-}O(2-)\text{-}\kappa O)(H_2O)_4]$;[20] XXII, $[Co[Ado\text{-}\kappa O^{2'},\text{-}\kappa O^{3'}\text{-}1\text{-}O(2-)](H_2O)_4]$.



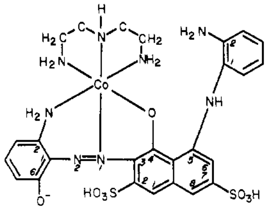
XXVI



XXVII



XXVIII



XXIX

XXVI, [3-[(2-amino-6-hydroxy-κO-phenyl)azo-κN^1]-5-[(2-aminophenyl)amino]-4-hydroxy-κO-2,7-naphthalenedisulfonato(2−)]-(diethylenetriamine-$\kappa^3 N$)cobalt(II)[19]
XXVII, [3-[(2-amino-6-hydroxy-κO-phenyl)azo-κN^2]-5-[(2-aminophenyl)amino]-4-hydroxy-κO-2,7-naphthalenedisulfonato(2−)]-(diethylenetriamine-$\kappa^3 N$)cobalt(II)
XXVIII, [3-[(2-amino-6-hydroxyphenyl)azo]-5-[(2-amino-κN-phenyl)amino-κN]-4-hydroxy-κO-2,7-naphthalenedisulfonato-(2−)](diethylenetriamine-$\kappa^3 N$)cobalt(II)
XXIX, [3-[(2-amino-κN-6-hydroxyphenyl)azo-κN^1]-5-[(2-aminophenyl)amino]-4-hydroxy-κO-2,7-naphthalenedisulfonato(2−)]-(diethylenetriamine-$\kappa^3 N$)cobalt(II)

Conclusions

We have proposed that the present use of atomic symbol locants to indicate donor atoms for ambidentate and flexidentate ligands be modified and applied with the highly successful *hapto* notation to provide a simple, obvious, and topologically exact notation for coordination compounds.

The Greek letter kappa (κ) is placed after the portion of the ligand name to which it applies in order to call attention to the fact that the ligating atom is to be identified. The ligating atom is identified by the italic element symbol, immediately after κ. The position of the ligating atom is indicated, where necessary, by a right superscript to the element symbol. Right superscripts are also used as multiplicative indexes by placing them on κ. Minor changes are proposed in the use of the *hapto* notation to indicate delocalized binding to groups of atoms. The Greek letter eta (η) is placed after the name of the grouping (as is κ) and a right superscript is used to indicate the number of points of attachment to the coordination center. When appropriate, locants are cited before eta and connected to it by a hypen with both locants and eta enclosed in parentheses. The two conventions, when combined, make possible the exact designation of modes of chelation in stuctures of much complexity.

Acknowledgment. The authors with to thank Dr. Warren H. Powell for much helpful discussion in the development of the material presented herein.

References and Notes

(1) F. Basolo, J. L. Burmeister, and A. J. Poe, *J. Am. Chem. Soc.*, **85**, 1700 (1963).
(2) W. J. Stratton and D. H. Busch, *J. Am. Chem. Soc.*, **80**, 3191 (1958).
(3) *Chem. Eng. News*, **28** (8), 520 (1948).
(4) "IUPAC, Nomenclature for Inorganic Chemistry (1957)", Butterworths, London, 1959.
(5) "IUPAC, Nomenclature for Inorganic Chemistry (1970)", 2nd ed, Butterworths, London, 1971.
(6) "The Naming and Indexing of Chemical Substances for *Chemical Abstracts* during the Ninth Collective Period (1972-1976)", ¶215, p 1021, a reprint of Section IV of the "Introduction to the Chemical Abstracts Volume 76 Index Guide".
(7) Private communication.

(8) Private communication.
(9) We have chosen not to use polynuclear examples because they would require us to present an ad hoc numbering for coordination centers in polynuclear compounds. Long experience in organic ring nomenclature and boron cluster numbering has indicated to us that great mischief in communication can and will occur when several numbering systems are simultaneously in use. Therefore, despite the temptation to forge our own proposals, prudence requires that this fundamental question should more appropriately be considered a separate issue.
(10) The more systematic index names are tris[2-pyridinecarboxyaldehyde-κN (2-pyridinylmethylene)hydrazone-κN^{1}]iron(2+) and bis[2-pyridinecarboxaldehyde-κN (2-pyridinyl-κN-methylene)hydrazone-κN^{1}]iron(2+). By inspection of these systematic index names, it is evident that the kappa infix atomic symbol locant fits even more naturally into the extended multipart ligand names than those based on more traditional nomenclature.
(11) F. A. Cotton, *J. Am. Chem. Soc.*, **90**, 6230 (1968).
(12) "IUPAC, Nomenclature for Inorganic Chemistry (1970)", 2nd ed, Butterworths, London, 1971, Rule 7.42 and Table III, p 103.
(13) Reference 12.
(14) H. Tom Dick and A. Orloppa, *Angew. Chem., Int. Ed. Engl.*, **14**, 251 (1975).
(15) -$\kappa N,\kappa N'$ could also be used to indicate the nitrogen chelation in [*N*,*N'*-ethanediylidenebis(isopropylamine)].
(16) R. B. King, *J. Organomet. Chem.*, **100**, 111 (1975).
(17) R. B. King and K. N. Chen, *Inorg. Chem.*, **16**, 1164 (1977).
(18) R. St. L. Bruce, M. K. Cooper, and B. G. McGrath, *J. Chem. Soc. D*, **2**, 69 (1970).
(19) -$\kappa N^{1},\kappa N^{4},\kappa N^{7}$ could also be used as the ligand locants for diethylenetriamine.
(20) Ado-1-O = adenosine 1-oxide.

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The Designation of Coordinating Sites in Ligands

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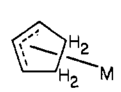
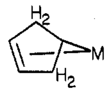
An alternative method to that described in the previous paper for designating coordinating sites in ligands is described. It supersedes the η system but, like it, uses a single designator, Ω. The method is particularly suitable for naming small polynuclear complexes.

Introduction

The problem of the designation of coordinating sites in ligands has been recognized for many years, and specific devices for dealing with it have been suggested by the Commission for the Nomenclature of Inorganic Chemistry of IUPAC (the use of italicized donor-element symbols with appropriate locants and primes)[1,2] and by Cotton (the "*hapto*" or η convention).[3] The use of italicized element symbols is not necessarily adequate when very complex ligands are involved and is incapable of dealing with situations in which more than one metal atom may bind to the same complex ligand. The "*hapto*" convention of Cotton, as adopted by IUPAC,[2] has been used in part more loosely than intended and in some ways more restrictively. For example, it was clearly intended by IUPAC that the convention should apply to sets of contiguous donor atoms of any kind, not just to carbon. The term "*monohapto*" is widely current, though this is a misnomer in IUPAC terms.[2] There is a clear need for a convention to allow the designation of "*monohapto*" coordination and to allow a distinction between (*trihapto*?) situations such as shown in structures a and b.



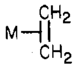
a



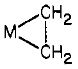
b

For this reason Busch and Sloan,[4] extending an idea due to Lozac'h[5] and Gustafson,[6] introduced the κ convention for designating simple coordination sites. The format they propose is sensible but the convention introduces a misleading concept and is limited in its description of multinuclear systems.

It misleads in that it implies a difference in bond type which is designated by η and κ which is not justified. In usage, η is generally understood to imply electron delocalization over several carbon atoms, though whether this really occurs is often a matter of subjective opinion rather than chemical discussion. However, there is no difference in principle between the binding of two carbon atoms to a metal as in structures c, d, or e, or even in f, g, or h. Should structures c and h be designated by η and structures e and f by κ or is the distinction unnecessary? In short, two symbols are superfluous, and possibly misleading. A single designator is sufficient, and avoids arguments over electron delocalization.[7]



c



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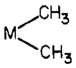
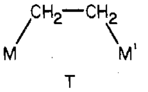


e



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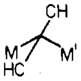

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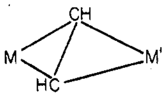

h

The η/κ symbolism is inadequate in that in polynuclear species it may be necessary to define which ligand atoms are bound to which metals. Neither the η nor the κ convention enables one to do this.

To overcome the above objections, I wish to propose an extension, which I name the Ω convention[8] which is at once both more flexible and more widely applicable than either κ or η, separately or together. The formating procedure closely follows that for κ,[4] upon which it is based.

The Ω Convention

(a) Single Ligand Atoms in Polyatomic Ligands. These are denoted by the italic element symbol of the ligand atom preceded by the Greek letter Ω. This is placed directly after that part of the ligand name in which the ligating group is contained. Any locants, primes, etc., needed to identify the ligand atom uniquely are indicated by superscripts to the italic element symbol. The Ω designator is separated from the conventional part of the name by a hyphen.

(b) More Than One Nonadjacent Single Ligand Atom in Polyatomic Ligands. When there is more than one ligand atom in the ligand, each ligand atom is cited in the name as in (a). Where two ligand atoms are cited in the same part of the name, they are written in the order of Table IV of the IUPAC

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