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COMMISSION ON NOMENCLATURE OF INORGANIC CHEMISTRY*

NOMENCLATURE OF INORGANIC CHAINS AND RING COMPOUNDS

(IUPAC Recommendations 1997)

Prepared for publication by

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Nomenclature of inorganic chain and ring compounds (IUPAC Recommendations 1997)

Abstract: In this document a systematic, additive approach to name inorganic chain and cyclic compounds is introduced. The method does not require any prior knowledge about the nature of bonds between the atoms. Though the method can be applied to all compounds, its use is mainly intended for inorganic compounds which are mainly composed of atoms other than carbon. In the case of neutral chain frameworks the compound is called "catena" preceded by a multiplicative prefix "di-", "tri-", etc. to indicate the number of branches in the molecule. Likewise cyclic compounds are called "cycle" preceded by the appropriate multiplicative prefix. A mixed chain and ring compound is named as "catenacycle". In the case of charged species the names are modified by the suffixes "-ium" and "-ate". The connectivity in the framework is indicated by a nodal descriptor which is placed in square brackets immediately before the terms "catena", "cycle" or "catenacycle". In simple chain and ring compounds it is permissible to replace the nodal descriptor with a numeric indicator [*n*] where *n* is the number of atoms in the principal chain or ring. The atoms are numbered according to the general nodal nomenclature regardless of their chemical identity. Only in the case of ambiguity is the chemical nature of the atoms taken into consideration. The atoms forming the nodal skeleton are listed in alphabetical order complete with their locants and are named by modifying the element radical names in TableVII of "Nomenclature of Inorganic Chemistry" (1) by substituting "-y" for the terminal "-io". Atoms and groups of atoms which are not a part of the nodal framework are named as ligands and are cited in alphabetical order together with their locants before the cited sequence of the atoms constituting the nodal framework.

INTRODUCTION

The development of the nomenclature for inorganic chain ring compounds has seen a long history. This history has recently been reviewed by Haiduc (2) and by Powell and Sloan (3). This document is concerned with a new systematic approach for the naming of inorganic chain and ring compounds that has been formulated after more than a decade of discussions and adjustments at annual meetings of the Commission on Nomenclature of Inorganic Chemistry.

The naming system presented below is based on additive nomenclature and thus does not require any prior knowledge about the nature of bonds between the atoms. Though the method can be applied to all compounds, its use is intended for inorganic compounds which are mainly composed of atoms other than carbon.

A neutral chain compound is called a "catena" and a neutral cyclic compound a "cycle". The corresponding cations are called "catenium" and "cyclium" and the anions "catenate" and "cyclate". The number of atoms in the chain or in the ring is given by a descriptor [*n*] placed immediately before the term "catena" or "cycle" and preceded by a hyphen.

Specific rules are needed for the selection and numbering of the principal chain or ring in the molecule. The elements which constitute the chain or ring framework are listed in alphabetical order complete with their locants and are named modifying the element radical names given in "Nomenclature of Inorganic Chemistry" (1) by substituting the terminal "-io" by "-y" (see Table 1). All atoms (including hydrogen) or groups of atoms which are not a part of the chain or ring framework are named as ligands. They are also listed in alphabetical order before the cited sequence of the chain or ring atom terms.

TABLE 1 The Names of The Elements Constituting The Principal Chain

Ac	actiny	Gd	gadoliny	Po	polony
Ag	argenty	Ge	germy *	Pr	praseodymy
Al	aluminy	H	hydrony **	Pt	platiny
Am	americy	He	hely	Pu	plutony
Ar	argony	Hf	hafny	Ra	rady
As	arsy *	Hg	mercury	Rb	rubidy
At	astaty	Ho	holmy	Re	rheny
Au	aury	I	iody	Rh	rhody
B	bory	In	indy	Ru	rutheny
Ba	bary	Ir	iridy	S	sulfy *
Be	berylly	K	potassy (kaly)	Sb	stiby
Bi	bismy *	Kr	kryptony	Sc	scandy
Bk	berkely	La	lanthany	Se	seleny
Br	bromy	Li	lithy	Si	sily *
C	carby **	Lr	lawrency	Sm	samary
Ca	calcy	Lu	lutety	Sn	stanny
Cd	cadmy	Md	mendelevy	Sr	stronty
Ce	cery	Mg	magnesy	T	trity
Cf	californy	Mn	mangany	Ta	tantaly
Cl	chlory	Mo	molybdy	Tb	terby
Cm	cury	N	azy **	Tc	technety
Co	cobalty	Na	sody (natry)	Te	tellury
Cr	chromy	Nb	nioby	Th	thory
Cs	caesy	Nd	neodymy	Ti	titany
Cu	cupry	Ne	neony	Tl	thally
D	deutery	Ni	nickely	Tm	thuly
Dy	dysprosy	No	nobely	U	urany
Er	erby	Np	neptuny	V	vanady
Es	einsteiny	O	oxy **	W	wolframy
Eu	europy	Os	osmy	Xe	xenony
F	fluory	P	phosphy	Y	yttry
Fe	ferry	Pa	protactiny	Yb	ytterby
Fm	fermy	Pb	plumby	Zn	zincy
Fr	francy	Pd	pallady	Zr	zircony
Ga	gally	Pm	promethy		

* The names do not derive directly from the radical names. ** There are no radical names for these elements.

UNBRANCHED CHAIN AND MONOCYCLIC COMPOUNDS

Chain compounds

General

In some cases it is convenient to treat the chain compound as unbranched. The molecules can then be described by defining a principal chain. Any branches attached to the principal chain are named as ligands. The number of atoms in the principal chain is given by a descriptor [*n*] placed immediately before the term "catena" and preceded by a hyphen. Thus, a six-membered chain is a -[6]catena. The chain-length is defined as the longest chain of atoms in the molecule, disregarding terminal hydrogen atoms. Terminal hydrogen atoms are named as ligands.

Example:

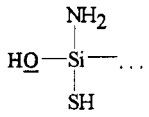
1. HS-S-S-SH
1,4-dihydridotetrasulfy-[4]catena

Choice of Principal Chain

If a penultimate chain atom is bound to more than one atom different from hydrogen, the terminal atom chosen is the one first encountered in the element sequence [Table IV; Red Book, Part 1 (1)].

Example:

1.

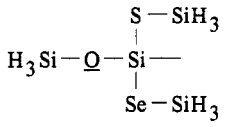


Oxygen stands first in the sequence and is preferred to sulfur and nitrogen. Therefore, O is a part of the chain.

If the terminal atoms of branched chains are identical, the choice of the principal chain is decided by comparison of the penultimate atoms or, if these also are identical, at the first point of difference moving inwards.

Example:

2.

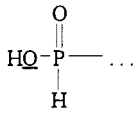


O is preferred to S and Se.

If the penultimate atom is bound to two identical atoms or the branches contain identical sequences of atoms but differ in the coordination numbers of some of the atoms the principal chain contains the element with higher coordination number.

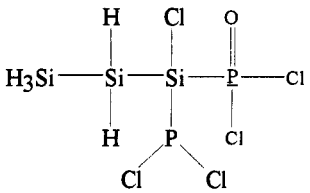
Examples:

3.



Oxygen with coordination number 2 is preferred to oxygen with coordination number 1.

4.



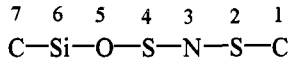
Phosphorus with coordination number 4 is preferred to phosphorus with coordination number 3.

Numbering of Chains

The chain is numbered from that end which assigns a lower locant, at the first point of difference, to the element first encountered in the sequence [Table IV; Red Book, Part 1 (1)].

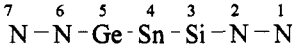
Examples:

1.



The direction of numbering is governed by the choice of atom in position 2. S is preferred to Si.

2.

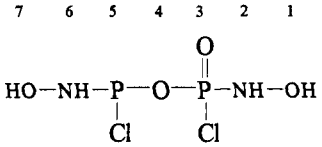


The direction is governed by the choice of atom in position 3. Si is preferred to Ge.

In chains which are symmetrical with respect to the central atom(s) the chain is numbered from that end which assigns a lower locant, at the first point of difference, to the element with the highest coordination number. In the case of equal coordination numbers the ligands appearing first in the element seniority sequence [Table IV; Red Book, Part 1 (1)] have preference. In the case of polyatomic ligands the first differing atom appearing first in element seniority sequence has preference.

Example:

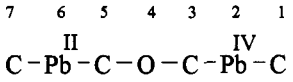
3.



Points of difference are also atoms of an element in different oxidation states. The atom in the higher oxidation state is preferred to the atom in the lower oxidation number.

Example:

4.



Pb^{IV} is preferred to Pb^{II}.

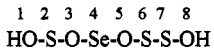
Construction of the Name

The name of a principal chain is constructed by citation of a series of "y" terms indicating the presence of each atom in the chain. The "y" terms are arranged alphabetically and provided with locants and multiplying prefixes, di-, tri-, tetra-, etc., as appropriate. All atoms or groups of atoms that are not considered as a part of the

principal chain (including hydrogen) are named as ligands according to coordination nomenclature principles and listed together with their locants in alphabetical order before the cited sequence of chain atom terms. Side chains consisting of common hydrocarbon substituents are denoted by customary substituent names, e.g., methyl.

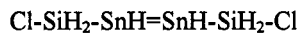
Examples:

1.



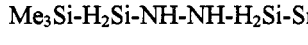
1,8-dihydrido-1,3,5,8-tetraoxy-4-seleny-2,6,7-trisulfy-[8]catena

2.



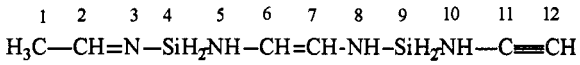
2,2,3,4,5,5-hexahydrido-1,6-dichlory-2,5-disily-3,4-distanny-[6]catena

3.



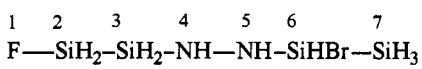
1,1,1,3,3,4,5,6,6,8,8,8-dodecahydrido-2,2,7,7-tetramethyl-4,5-diazy-1,8-dicarby-2,3,6-trisily-7-stanny-[8]catena

4.



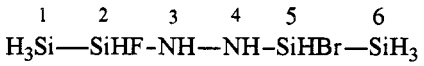
1,1,1,2,2,4,4,5,6,7,8,9,9,10,12-pentadecahydrido-3,5,8,10-tetraazy-1,2,6,7,11,12-hexacarby-4,9-disily-[12]catena

5.



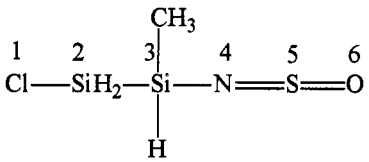
6-bromo-2,2,3,3,4,5,6,7,7,7-decahydrido-4,5-diazy-1-fluory-2,3,6,7-tetrasily-[7]catena

6.



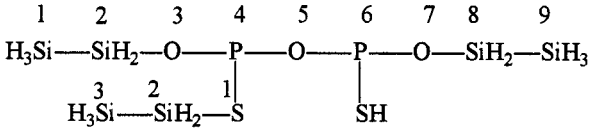
5-bromo-2-fluoro-1,1,1,2,3,4,5,6,6,6-decahydrido-3,4-diazy-1,2,5,6-tetrasily-[6]catena

7.



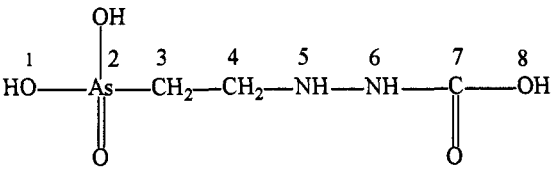
2,2,3-trihydrido-3-methyl-4-azy-1-chlory-6-oxy-2,3-disily-5-sulfy-[6]catena

8.



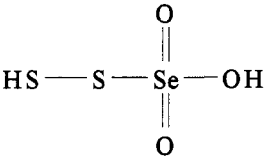
1,1,1,2,2,8,8,9,9,9-decahydrido-4-{2,2,3,3,3-pentahydrido-2,3-disily-1-sulfy-[3]caten-1-ato}-6-sulfanido-3,5,7-trioxy-4,6-diphosphy-1,2,8,9-tetrasily-[9]catena

9.



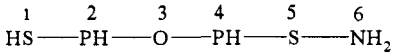
1,3,3,4,4,5,6,8-octahydrido-2-hydroxo-2,7-dioxo-2-arsy-5,6-diazy-3,4,7-tricarby-1,8-dioxy-[8]catena

10.



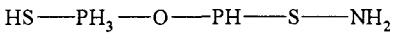
1,4-dihydrido-2,2-dioxo-1-oxy-2-seleny-3,4-disulfy-[4]catena

11.



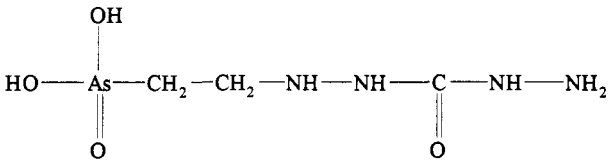
1,2,4,6,6-pentahydrido-6-azy-3-oxy-2,4-diphosphy-1,5-disulfy-[6]catena

12.



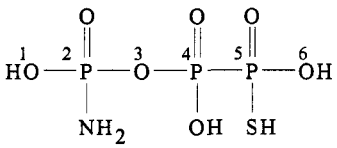
1,2,2,2,4,6,6-heptahydrido-6-azy-3-oxy-2,4-diphosphy-1,5-disulfy-[6]catena

13.



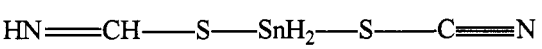
1,3,3,4,4,5,6,8,9,9-decahydrido-2-hydroxo-2,7-dioxo-2-arsy-5,6,8,9-tetraazy-3,4,7-tricarby-1-oxy-[9]catena

14.



2-amido-1,6-dihydrido-4-hydroxo-2,4,5-trioxo-5-sulfanido-1,3,6-trioxy-2,4,5-triphosphy-[6]catena

15.



1,2,4,4-tetrahydrido-1,7-diazy-2,6-dicarby-4-stanny-3,5-disulfy-[7]catena

When metal atoms are present in the chain, their oxidation states should be given according to STOCK's

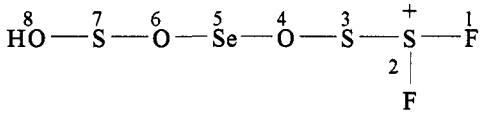
system, i.e. the oxidation number of the metal is indicated by a Roman numeral placed in parenthesis immediately following the name of the element. For zero the cipher 0 is used. Examples are chromy(II), chromy(III), chromy(0), etc. When used in conjunction with symbols the Roman numeral is placed above and to the right.

Cations

Chain cations are named "catenium"-ions. The charge of the cation indicated by an Arabic numeral followed by the plus sign is placed in parenthesis following the ending "ium" (EWENS-BASSETT system). The location of the charge in the backbone of the chain may be indicated by a locant before the ending -ium.

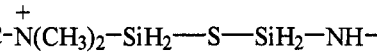
Examples:

1.



2-fluoro-8-hydrido-1-fluory-4,6,8-trioxy-5-seleny-2,3,7-trisulfy-[8]catenium(1+)
or
2-fluoro-8-hydrido-1-fluory-4,6,8-trioxy-5-seleny-2,3,7-trisulfy-[8]caten-2-ium(1+)

2.



1,1,1,3,3,5,5,6,7,7,7-undecahydrido-2,2-dimethyl-2,6-diazy-1,7-dicarby-3,5-disily-4-sulfy-[7]catenium(1+) bromide
or
1,1,1,3,3,5,5,6,7,7,7-undecahydrido-2,2-dimethyl-2,6-diazy-1,7-dicarby-3,5-disily-4-sulfy-[7]caten-2-ium(1+) bromide

If the position of the positive charge of a catenium ion is uncertain, it is simply designated a catenium ion:

Examples:

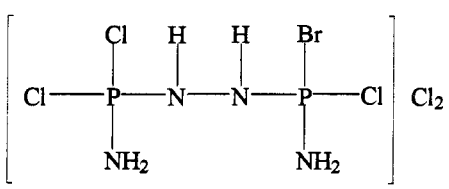
3. $[H_2N\text{-}PPh_2\text{-}N\text{-}PPh_2\text{-}NH_2]Cl$

1,1,5,5-tetrahydrido-2,2,4,4-tetraphenyl-1,3,5-triazy-2,4-diphosphy-[5]catenium(1+) chloride

4. $[Cl\text{-}P(NH_2)Cl\text{-}N\text{-}P(NH_2)Cl\text{-}Cl]\ Cl$

2,4-diamido-2,4-dichloro-3-azy-1,5-dichlory-2,4-diphosphy-[5]catenium(1+) chloride

5.



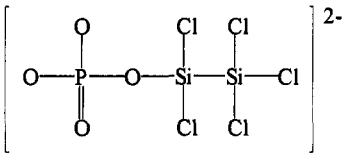
2,5-diamido-5-bromo-2-chloro-3,4-dihydrido-3,4-diazy-1,6-dichlory-2,5-diphosphy-[6]catenium(2+) dichloride

Anions

Chain Anions. Chain anions are named "catenate"-ions. The charge of the anion indicated by an Arabic numeral followed by the minus sign is placed in parenthesis following the ending "ate" (EWENS-BASSETT system). The location of the charge in the backbone of the chain may be indicated by a locant before the ending -ate.

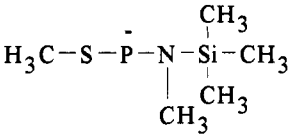
Examples:

1.



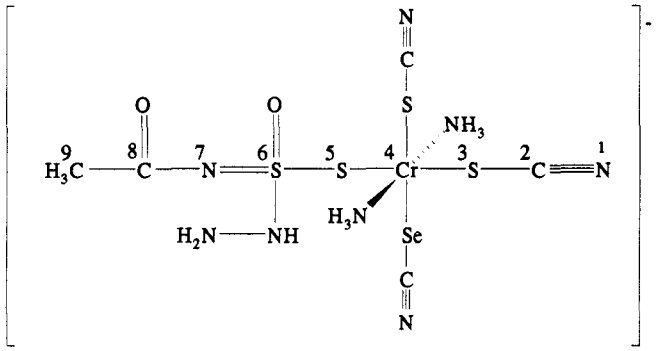
2,2,3,3-tetrachloro-5,5-dioxo-1-chlory-4,6-dioxy-5-phosphy-2,3-disily-[6]catenate(2-)

2.



1,1,1,6,6,6-hexahydrido-4,5,5-trimethyl-4-azy-1,6-dicarby-3-phosphy-5-sily-2-sulfy-[6]caten-3-ate(1-)

3.



4,4-diammine-6-hydrazido-9,9,9-trihydrido-6,8-dioxo-4-selenocyanato-4-thiocyanato-1,7-diazy-2,8,9-tricarby-4-chromy(III)-3,5,6-trisulfy-[9]catenate(1-)

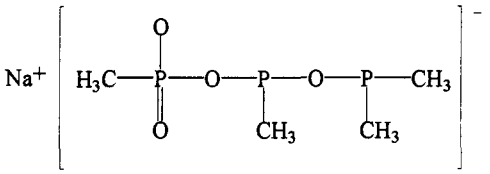
or

4,4-diammine-4-(3-azy-2-carby-1-seleny-[3]-caten-1-ato)-4-(3-azy-2-carby-1-sulfy-[3]caten-1-ato)-6-hydrazido-9,9,9-trihydrido-6,8-dioxo-1,7-diazy-2,8,9-tricarby-4-chromy(III)-3,5,6-trisulfy-[9]caten-4-ate(1-)

If the position of the negative charge of a catenate ion is uncertain, it is simply designated a catenate ion.

Example:

4.



sodium 1,1,1,7,7,7-hexahydrido-4,6-dimethyl-2,2-dioxo-1,7-dicarby-3,5-dioxy-2,4,6-triphosphy-[7]catenate.

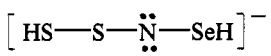
Anionic Ligand Name. Ligands derived from catenas by the loss of hydrons are given the ending -ato. The location of the charge may be indicated with a locant placed before the ending.

Examples:

1. $H_3Si\text{-}SiH_2\text{-}S\text{-}$

2,2,3,3,3-pentahydrido-2,3-disily-1-sulfy-[3]caten-1-ato

2.



1,4-dihydrido-3-azy-4-seleny-1,2-disulfy-[4]caten-3-ato

Radicals

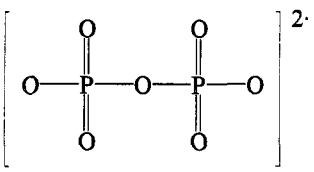
Radicals are named by adding the ending "-yl", "-diyl", etc. to the name of the catena or catenate, with elision of terminal "a" or "e" (catenate) when followed by "y", preceded by the locant of the atoms carrying the unpaired electron(s).

Examples:

1. $H_3Si\text{-}NH\text{-}NH\cdot$

1,2,3,3,3-pentahydrido-1,2-diazy-3-sily-[3]caten-1-yl

2.



2,2,4,4-tetraoxo-1,3,5-trioxy-2,4-diphosphy-[5]catenate(2-)-1,5-diyl

Monocyclic Compounds

The following nomenclature provides names for inorganic ring compounds consisting mainly of elements other than carbon. Ring systems containing two or more consecutive carbon atoms are usually named according to the rules of "Nomenclature of Organic Chemistry" (4).

A neutral monocyclic ring compound is called a "cycle", an anion a "cyclate"-ion, and a cation a "cyclium"-ion. The number of atoms in the ring is given by an indicator [*n*] placed immediately before the term "cycle", "cyclate", or "cyclium", and preceded by a hyphen. Thus, a six membered ring is a -[6]cycle. In order to emphasize the cyclic structure with the descriptor it is acceptable to use a zero before the Arabic number, i.e. -[06]cycle.

The names of derivatives of cycles are formed from the cycle name using coordination nomenclature [see chapters 7 and 10 in "Nomenclature of Inorganic Chemistry" (1)]. All ligands including hydrogen are named by coordination nomenclature and are listed in alphabetical order.

Numbering of Ring Atoms

Choice of Position One

(1) The elements which constitute the ring are named according to Table VII in "Nomenclature of Inorganic Chemistry" (1) by substituting the terminal "io" by "y" (see Table 1 in the present document) and listed in alphabetical order.

(2) Numbering starts at the atom which is listed first in Table IV of "Nomenclature of Inorganic Chemistry" (1).

(3) If two or more atoms of highest seniority are ring members, the one with the neighbour which follows next in Table IV (1) is the starting atom. If this second operation does not define a unique starting atom, neighbours once removed are sequentially considered, until a unique starting atom has been found or shown not to exist.

(4) If the above criteria fail to define unique starting atom, it is determined by consideration of the coordination numbers of those ring atoms which have the highest seniority in Table IV (1). The starting atom is the one with the highest coordination number. If needed, the coordination numbers of the neighbouring atoms are sequentially considered, until a unique starting atom has been found or shown not to exist.

(5) If the application of the above criteria identifies two or more equal contenders as starting atoms a choice must be made between them. Priority is given to the atom whose ligand comes first alphabetically.

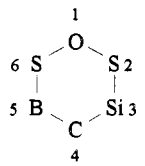
(6) If all ligands are equal, the ligands on neighbours once removed are sequentially considered, until a unique starting atom has been found. If no unique starting atom is found by this method, the symmetry of the ring and its ligands is such that an arbitrary choice will lead to a unique name. The starting atom may be arbitrarily chosen from among the equal contenders for priority.

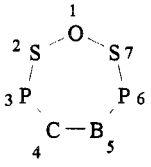
Direction of Numbering. This is determined by application of the following criteria in order until a decision is reached:

(1) The direction of numbering leads from position 1 to whichever neighbouring atom is listed first in Table IV (1).

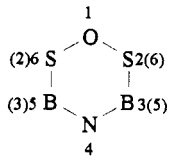
(2) If both neighbouring atoms are the same, the pair of next nearest neighbours are compared, until a unique atom first in Table IV (1) is identified.

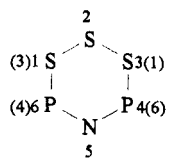
Unique numbering





Alternative numbering as shown in parentheses.





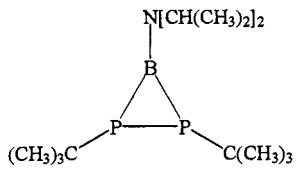
(3) When the direction of numbering cannot be determined by considering the ring atoms it is determined by considering the ligands. The direction of numbering leads from the starting atom to a neighbour with a ligand.

(4) If both have ligands it leads to that whose ligand comes first alphabetically.

(5) If the ligands are equal, the ligands on next nearest neighbours are considered and so on until a unique direction is attained. If none is found the symmetry of ring and ligands leads to unique name independently of the direction.

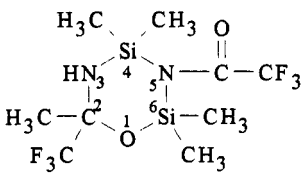
Examples:

1.



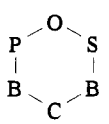
1,2-di-*tert*-butyl-3-diisopropylamino-3-bory-1,2-diphosphy-[3]cycle

2.

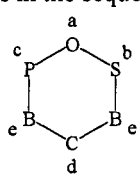


3-hydrido-2,4,4,6,6-pentamethyl-5-trifluoroacetyl-2-trifluoromethyl-3,5-diazy-2-carby-1-oxy-4,6-disily-[6]cycle

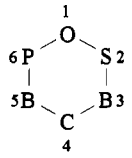
Procedure of Numbering. In order to facilitate numbering, the ring members in a given system can be alphabetically labeled to indicate their relative position in the sequence of Table IV (1).



The relative positions in the sequence of elements are as follows:

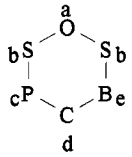


For numbering, that direction is chosen which gives the initial sequence of letters earliest in the alphabet. The resulting sequence a,b,e,d,e,c leads to the numbering



If the "initial" atom in the ring has neighbours of the same kind on both sides, that sequence is preferred which contains the second or subsequent sequence of letters earliest in the alphabet.

In



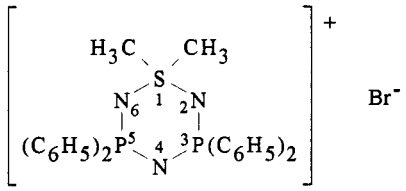
the sequence is a,b,c,d,e,b rather than a,b,e,d,c,b.

Cationic Monocyclic Ring Compounds

Cyclic inorganic cations are named in the same way as the neutral ring systems, but instead of "cycle" the suffix "cyclium" is used. A locant for the charge may be inserted before "ium".

Example:

1.



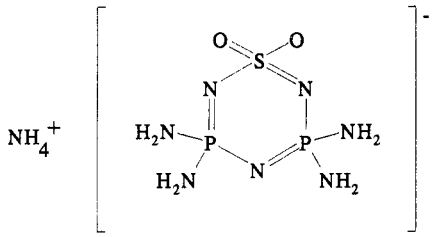
1,1-dimethyl-3,3,5,5-tetraphenyl-2,4,6-triazy-3,5-diphosphy-1-sulfy-[6]cyclium bromide

Anionic Monocyclic Ring Compounds

Cyclic inorganic anions are named in the same way as the neutral ring systems, but instead of "cycle" the suffix "cyclate" is used. A locant for charge may be inserted before "ate".

Example:

1.

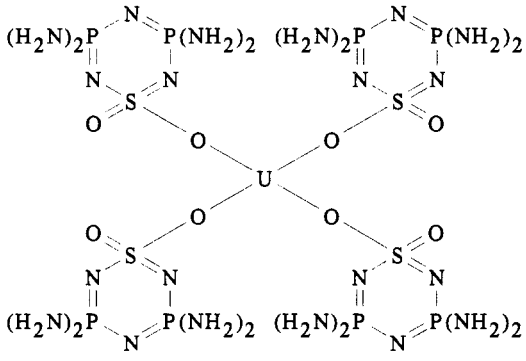


ammonium 3,3,5,5-tetraamido-1,1-dioxo-2,4,6-triazy-3,5-diphosphy-1-sulfy-[6]cyclate

When an anionic monocyclic ring acts as a ligand, its name is modified by replacing the ending "ate" by "ato".

Example:

2.



tetrakis(3,3,5,5-tetraamido-1,1-dioxo-2,4,6-triazy-3,5-diphosphy-1-sulfy-[6]cyclato)uranium(IV)

BRANCHED CHAIN AND POLYCYCLIC COMPOUNDS

Introduction

The method described above can conveniently be extended to chain compounds containing more complicated branched structures, to polycyclic compounds, and to mixed chain and ring compounds by use of the general nodal descriptor (5).

Nodal nomenclature has originally been developed to solve problems encountered in naming complicated organic molecules. It is based on the description of the structure of a molecule in terms of its graph. Each graph is thought to be composed of one or more modules which are defined as separate entities during the numbering and naming of the graph assembly. Each module in turn is composed of nodes that are the simplest units in the graph and represent either a single atom or a group of atoms (contraction nodes). The general nodal nomenclature defines rules by which the nodes of the graph are arranged and numbered. It differs from the standard organic nomenclature, because a unique numerical locant has to be provided for every node in the graph. At the most general level of treatment the nodal nomenclature does not specify the nature of the nodes or the bonding between them. Thus, it is not necessary to assume any specific ligancy for any node. Therefore nodal principles can equally well be applied for organic chemistry (6,7) and for inorganic chemistry (2,3). Nodal nomenclature is also shown to be useful when computerizing chemical nomenclature (8).

In the following, the basic rationale in the constructing of the nodal descriptor is summarized according to the concepts developed by Lozac'h, Goodson, and Powell (5) followed by their special application to branched chain and polycyclic inorganic systems.

The Nodal Descriptor

Basic Definitions

The modules of the graph (or the graph itself if there is only one module in the structure) can be acyclic, monocyclic or polycyclic.

(1) *An acyclic graph* (module) is an unbranched chain of nodes, or two or more unbranched chains of nodes connected to each other without formation of a cyclic structure.

(2) *A monocyclic graph* (module) is constructed when one end of the chain of nodes is attached to the other end forming only one ring in the structure.

(3) *A polycyclic graph* (module) consists of a monocyclic ring of nodes and one or more bridges which are valence bonds or chains of nodes connecting the nodes of the ring and/or other bridges in the polycyclic system.

(4) If a structure graph is composed of more than one cyclic module or of at least one acyclic and one cyclic module, it is called an *assembly*.

The Numbering of Nodes

General Considerations. Each node in the graph needs to be numbered. The general nodal nomenclature (5) provides detailed instructions on the relative seniority of the nodes regardless of their chemical identity. The chemical nature of the nodes is taken into consideration only to distinguish between two otherwise equivalent numberings.

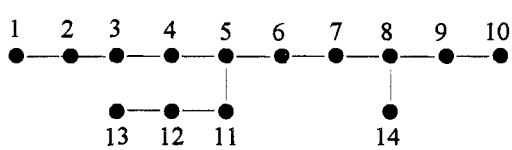
This is also the rationale to be followed in naming more complicated inorganic ring and chain compounds. The seniority is decided as far as possible using basic rules of general nodal nomenclature. The priority rules derived for the simple chain and monocyclic compounds which take into account the chemical nature of the elements according to the element seniority sequence {the element which comes first in the sequence has the higher seniority [see Table IV of the Red Book, Part 1 (1)]} are considered only when ambiguity arises.

Acyclic Graphs are characterized by a main chain which is defined as the longest unbranched chain of nodes. Terminal hydrogen atoms are not considered as a part of the chain. They are always named as ligands. If the penultimate atom is bound to more than one atom different from hydrogen, the terminal atom is chosen as the one first encountered in the element seniority sequence [see Table IV, Red Book, Part 1 (1)]. All other chains in the acyclic graph are defined as branches.

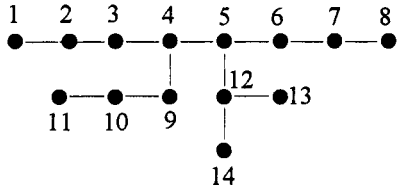
If there is more than one unbranched chain of the greatest length, the main chain is the one having the longest branch attached to it. The nodes in the main chain are numbered from one end to another so that the lowest possible locant is given to this branch of highest priority.* The branches are numbered in the order of their seniority (decreasing length) beginning from the node attached to the part of the graph already numbered.

Examples:

1.

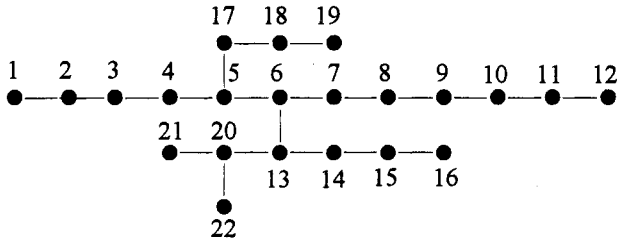


2.



In this case there are two possible main chains (1-2-3-4-5-6-7-8 and 11-10-9-4-5-6-7-8). The choice has to be made considering the element seniority sequence.

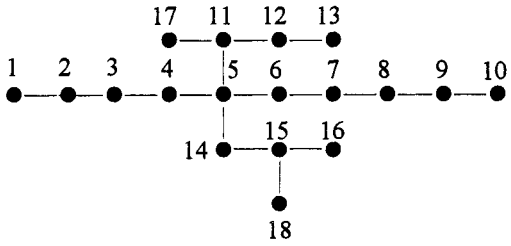
3.



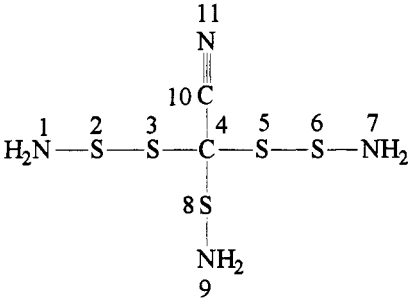
If alternative numberings remain, the choice is made by comparing the locants of the branches term by term in the order that the branches are numbered and selecting the lowest possible locants. Should any ambiguity still remain, it is resolved by considering the element seniority sequence.

Examples:

4.



5.



The principal chain is seven atoms long and its atoms are numbered starting from either nitrogen atom in the NH_2 groups. Since terminal hydrogen atoms are not considered as a part of the nodal framework, the two branches connected with the main chain are of equal length. However, S is senior to C in the element seniority sequence and thus the branch containing S is numbered first.

---

* Note that this practice is different in the nomenclature for simple chain compounds where only the main chain is included in the basic framework and the branches are named as ligands. It is then the element seniority sequence (Table IV; Ref. 1) which governs the choice of the main chain.

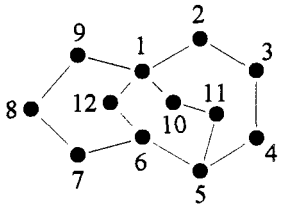
Monocyclic Graphs. The starting point and the direction of the numbering of the atoms in the monocyclic compound are determined by considering the chemical nature of the atoms constituting the ring or of the ligands attached to the ring according to the element seniority sequence as described above.

Polycyclic Graphs. A polycyclic graph is characterized by a main ring. Chains attached from both ends to the main ring are called bridges. The main ring in a polycyclic graph is defined as the monocyclic ring with the largest number of nodes. The main bridge is defined as the longest chain of nodes both ends of which are attached to the main ring. All other bridges are called secondary bridges. Note that a bridge can also be a bond in which case it contains no nodes.

The numbering of the main ring in the polycyclic graph begins at one of the bridgeheads (the node where the main bridge is attached to the main ring) and proceeds in the direction to give the lowest possible locant for the other bridgehead. The bridges are numbered sequentially after the main ring in the order of their seniority beginning always with the longest bridge connected to nodes of the graph previously numbered. Should there be two or more bridges of equal length, the one with lower locants has the higher seniority. The numbering of each bridge begins with the node connected to the node with the lower locant.

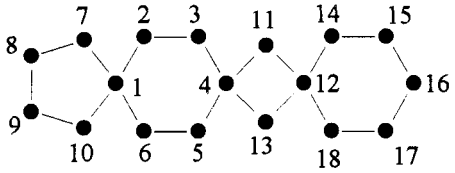
Examples:

1.



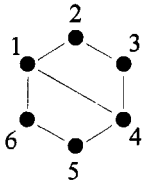
The main ring has nine nodes. The main bridge is the chain of two nodes connecting the nodes 1 and 5.

2.



Should there be two or more monocyclic rings having the largest number of nodes, the main ring is selected as the one having the main bridge with the greater number of nodes.

3.



The atoms 1 and 4 are connected by a bond and thus the main bridge contains no nodes.

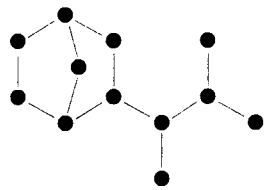
Assemblies. The definitive numbering of assemblies is carried out by numbering initially each module as if it were an isolated graph. The principal module and the seniority of the modules in assemblies are determined according to the successive application of the following criteria: (1) largest number of nodes; (2) a cyclic module preferred to an acyclic one; (3) largest number of rings or branches; (4) the descriptor with the

preferred Arabic numeral at the first difference: if the first difference corresponds to a chain or a bridge length, the preferred numeral is higher; if the first difference appears in a locant (superscript), the preferred numeral is lower.

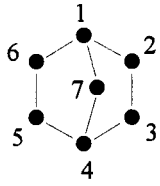
The original numbering is retained for the principal module. The numberings of nodes in all other modules are modified sequentially, beginning with a module adjoining the principal module (5). The renumbering is carried out by adding to each original locant a number equal to the total number of nodes in other modules that have already been assigned definitive locants.

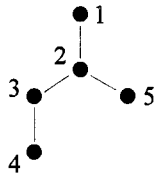
Example:

1.

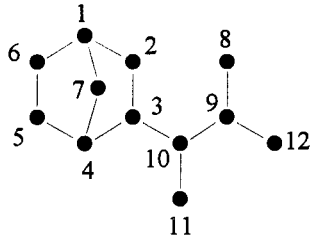


The molecule consists of one cyclic and one acyclic module which are initially numbered separately as follows:





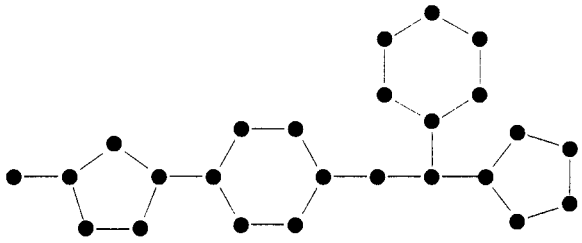
The cyclic module has a preference over the acyclic one and is thus the principal module in the graph. The numbering in the acyclic module is modified by adding 7 to each locant. The final definite numbering is accordingly the following:



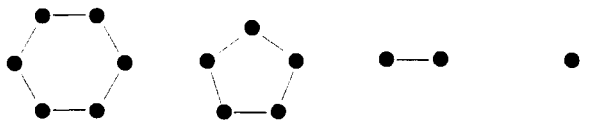
In some cases there are several renumbering schemes possible for the given assembly. The correct choice is made on the basis of a module seniority graph (5). In case of any remaining ambiguity the correct numbering has the lowest locants defining the attachments of the modules. In case of need the final resolution is made by considering the element seniority sequence.

Example:

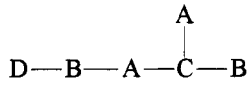
2.



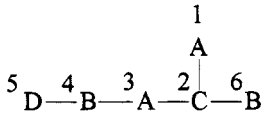
The graph consists of the following modules:



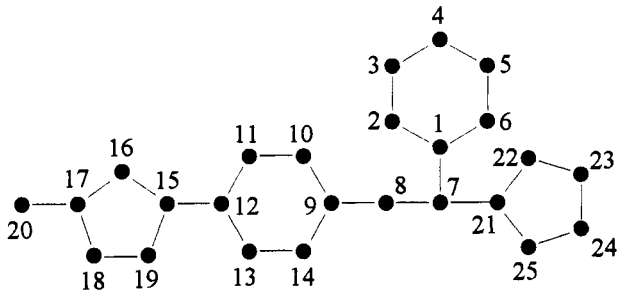
They are assigned module seniority descriptors A-D in the order of decreasing seniority. In effect, the letters A-D represent contraction nodes. Thus the module seniority graph of the molecule can be written as follows:



The modules are now numbered using the module seniority numbers. They begin with the principal module and proceed through the chain of modules in order of their decreasing seniority. The rules for assigning module seniority numbers are similar, but not analogous to the numbering of nodes in acyclic graphs (5):



The definitive numbering of the nodes in the whole assembly is now carried out in the order of the module seniority numbers (for more details of the definitive numbering of the assemblies, see Ref. 3).



Descriptor

The unambiguous description of the graph is provided by a descriptor. It is a numerical portion in the name and is placed in square brackets.

Acyclic Graphs. The descriptor of the acyclic graphs is constructed as follows:

(1) The descriptor of the acyclic graphs begins with an Arabic numeral indicating the number of the nodes in the main chain.* This portion of the descriptor ends with a period.

(2) The period is followed by positive Arabic numerals indicating the number of nodes in each branch cited in the order of their seniority.

(3) A superscript locant for each branch denotes the node in the part of the graph already numbered to which the branch is attached.

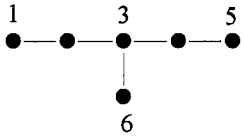
When it is possible to write alternative descriptors for the graph the correct one has the lowest superscript number at the first point of difference on term by term comparison.

Examples:

1.

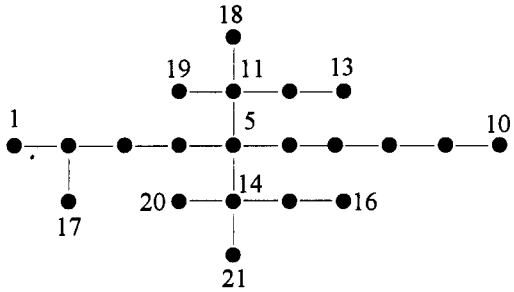
descriptor: [7]

2.



descriptor: $[5.1^3]$

3.

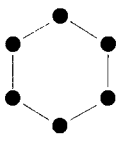


descriptor: $[10.3^5 3^5 1^2 1^{11} 1^{11} 1^{11} 1^{14} 1^{14}]$

Cyclic Graphs. The descriptor of the monocyclic graphs is an Arabic numeral indicating the number of nodes in the ring. The numeral is preceded by zero which indicates the presence of the ring.*

Example:

1.



descriptor: [06]

* If the nodal framework consists only of the main chain with all branches named as ligands, the nodal descriptor is identical with the indicator [*n*] used for the simple unbranched inorganic chain compounds.

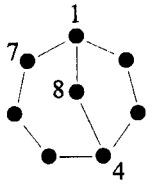
The descriptor for polycyclic graphs is constructed in analogous manner to that for branched graphs.

(1) The descriptor begins with a zero indicating the presence of a ring followed by an Arabic numeral indicating the number of nodes in the main ring. This portion of the descriptor ends with a period.
(2) The period is followed by Arabic numerals indicating the number of nodes in each bridge cited in the order of their seniority.
(3) A pair of superscript locants for each bridge numeral, separated by a comma and cited in increasing numerical order, denotes the nodes in the part of the graph already numbered to which each bridge is attached.

Should there be a choice for the main ring, main bridge, starting point and/or direction of numbering in the polycyclic graph, the Arabic numerals denoting the lengths and positions of the bridges in the various alternative descriptors are compared term by term in the order they appear. The descriptor with the preferred Arabic numeral at the first difference is chosen (in case of the bridge length, the preferred numeral is higher; in case of the locant, lower).

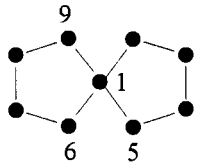
Examples:

2.



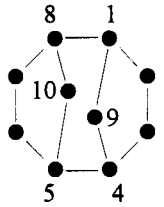
descriptor: [07.1^{1,4}]

3.



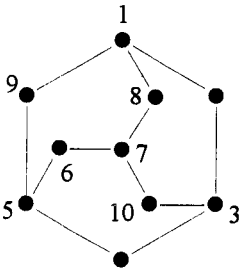
descriptor: [05.4^{1,1}]

4.



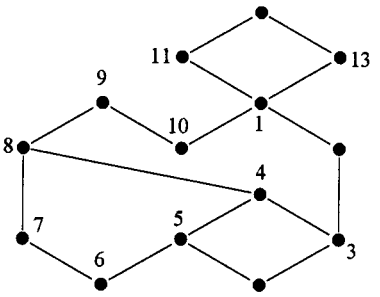
descriptor: [08.1^{1,4}1^{5,8}]

5.



descriptor: [08.1^{1,5}1^{3,7}]

6.



descriptor: [010.3^{1,1}1^{3,5}0^{4,8}]

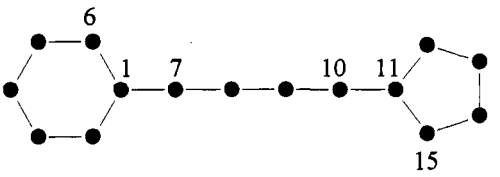
Assemblies. The assembly descriptor consists of square brackets enclosing, in the order of their seniority, the nodal descriptors of each module in parentheses and cited as if they were isolated graphs. Between the descriptors of the modules the locants of the nodes linking the modules are indicated. These locants are separated by a colon and are referred to by their definitive sequential numbering obtained when considering the whole assembly.

---

* In the nomenclature for the monocyclic compounds the zero is not a required part of the descriptor; its use is, however, permissible if the cyclic nature of the compound needs to be emphasized.

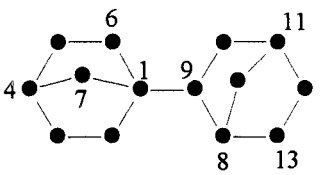
Examples:

1.



descriptor: [(06)1:7(4)10:11(05)]

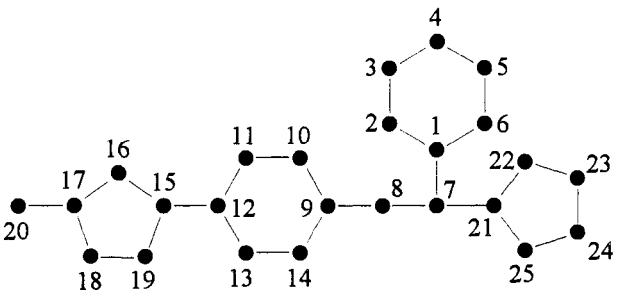
2.



descriptor: [(06.$1^{1,4}$)1:9(06.$1^{1,4}$)]

The descriptors for both modules are obtained as if the module were an isolated graph. The highest node in the principal module has the locant seven. The lowest locant (eight) of the second module is at the bridgehead as required by the numbering rules and not at the node where the modules are attached together. Thus it is possible to infer from the descriptor that the two parts of the molecule are identical, but attached to each other at different respective locations.

3.



descriptor: [(06)1:7(2)8:9(06)12:15(05)17:20(1)7:21(05)]

Construction of The Name

General Considerations

When naming the compound, it is important to decide which parts of the molecule should be included in the nodal skeleton. All other parts will be named as ligands.

If the nodal skeleton consists only of the main chain or of the main ring, the compounds are named following the nomenclature derived for umbranched chain and monocyclic compounds (see above).

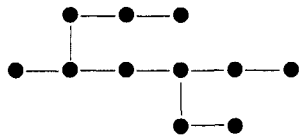
If the nodal skeleton is composed of a branched acyclic framework, the compound is called "catena" preceded by a multiplicative prefix "di-", "tri-", etc. to indicate the number of branches in the molecule. The cationic species are called "catenium" and the anionic species "catenate".

In an analogous manner a neutral polycyclic compound is called "cycle" preceded by a multiplicative prefix "di-", "tri-", etc. to indicate the number of rings in the molecule. The cationic species are called "cyclium" and the anionic species "cyclate".

If there are both cyclic and acyclic modules in the molecule the compound is named as "catenacycle" (the names are cited in alphabetic order) with both parts of the name preceded by appropriate multiplicative prefixes.

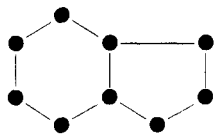
Examples:

1.



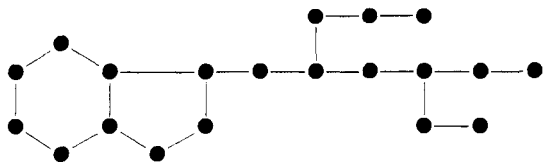
"tricatena"

2.



"dicycle"

3.



"tricatenadicycle"

Since the nodal descriptor only indicates the geometrical arrangement of the atoms, it is necessary to state unambiguously the chemical identity of each node. Following the practice introduced for the inorganic unbranched chain and monocyclic compounds the skeletal atoms forming the nodal framework are named modifying the radical names given in the Red Book (1) by substituting the terminal "-io" by "-y" (see also Table 1 in the present document). All atoms or groups of atoms which are not considered as a part of the polycyclic framework are named as ligands.

Ligands

In principle all atoms in the molecule can be treated as a part of the nodal framework. The resulting names will, however, become too cumbersome to be practical. Therefore it is preferable to name some atoms or groups of atoms as ligands to the nodal skeleton.

There are atoms or groups of atoms which are usually considered as ligands in coordination compounds. Some examples of typical ligands are given in Table 2. For more detailed treatment, see Chapter I-10 of "Nomenclature of Inorganic Chemistry" (1). It is also permissible to name any part of the molecule as a ligand if it is considered convenient in specific situations. There are, however, two restrictions in the use of the ligands in nodal frameworks:

(1) All ligands must be monodentate.
(2) The main chain in acyclic modules can only be terminated by a ligand if the ligand is either a hydrogen atom or an organic fragment.

Table 2. Examples of typical ligands *

Ligand	Name	Ligand	Name
F^-	fluoro	CH_3	methyl
Cl^-	chloro	CH_3CH_2	ethyl
Br^-	bromo	$CH_3CH_2CH_2$	propyl
I^-	iodo	$(CH_3)_3C$	1,1-dimethylethyl (*tert*-butyl)
CO	carbonyl	C_5H_5	cyclopentadienyl
NCO^-	cyanato	C_6H_5	phenyl
Ph_3P	triphenylphosphane		

The Name Construction

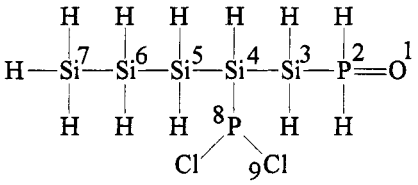
The name consists of the following parts:

(1) Ligands listed in alphabetic order complete with their definitive sequential locants.
(2) Skeletal atoms forming the nodal framework listed in alphabetic order together with their definitive sequential locants when needed.
(3) The nodal descriptor in square brackets.
(4) The designator "catena", "cycle", or "catenacycle" for neutral molecules, "catenium", "cyclium", or "catenacyclium" for cations, and "catenate", "cyclate", or "catenacyclate" for anions, preceded by appropriate multiplicative prefixes.

Branched Acyclic Compounds.

Examples:

1.



2,2,3,3,4,5,5,6,6,7,7,7-dodecahydrido-9,10-dichlory-1-oxy-2,8-diphosphy-3,4,5,6,7-pentasily-[7.2^41^8]tricatena

* See Tables I-10.1, I-10.2, I-10.3, I-10.4, and I-10.9 (1) for additional examples.

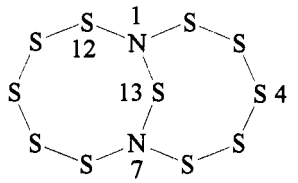
It might be preferable to name the two chlorine atoms as ligands in orde to emphasize that they are identically bound to P(8). The name would thus be:

8,8-dichloro-2,2,3,3,4,5,5,6,6,7,7,7-dodecahydrido-1-oxy-2,8-diphosphy-3,4,5,6,7-pentasily-[7.1^4]dicatena

Polycyclic Compounds

Examples:

1.

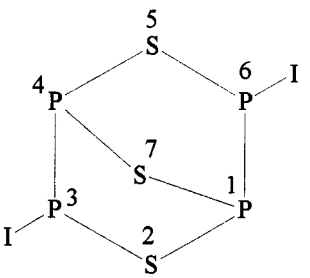


1,7-diazy-2,3,4,5,6,8,9,10,11,12,13-undecasulfy-[012.1^{1,7}]dicycle

Since the compound contains only nitrogen and sulfur, it is not necessary to indicate the locants of all sulfur atoms. Only the locants of the two nitrogen atoms are needed.

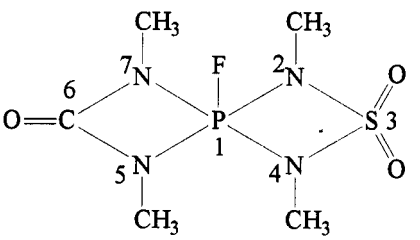
1,7-diazyundecasulfy-[012.1^{1,7}]dicycle

2.



3,6-diiodo-1,3,4,6-tetraphosphy-2,5,7-trisulfy-[06.1^{1,4}]dicycle

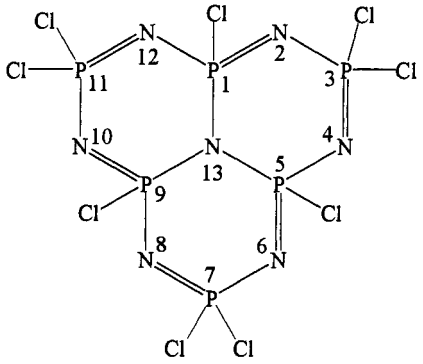
3.



1-fluoro-2,4,5,7-tetramethyl-3,3,6-trioxo-2,4,5,7-tetraazy-6-carby-1-phosphy-3-sulfy-[04.3^{1,1}]dicycle

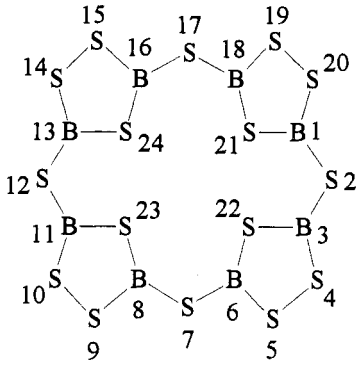
Phosphorus has the locant 1. As the nodal framework comprises only the seven atoms forming the two rings with other groups named as ligands, it is not possible to select the main ring unambiquously by considering only the graph of the molecule. The selection of the main ring is determined by the fact that sulfur is senior to carbon according to the element seniority sequence (1).

4.



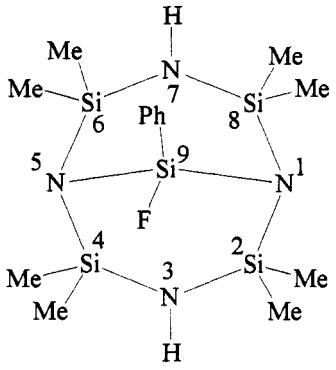
1,3,3,5,7,7,9,11,11-nonachloro-2,4,6,8,10,12,13-heptaazy-1,3,5,7,9,11-hexaphosphy-[012.1^{1,5}0^{9,13}]tricycle

5.



1,3,6,8,11,13,16,18-octaboryhexadecasulfy-[020.1^{1,18}1^{3,6}1^{8,11}1^{13,16}]pentacycle

6.

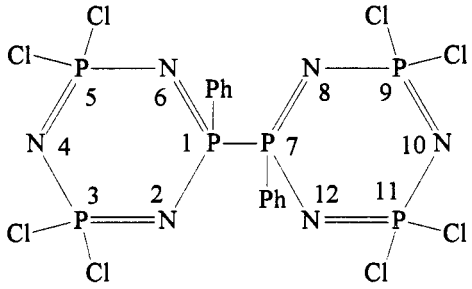


9-fluoro-3,7-dihydrido-2,2,4,4,6,6,8,8-octamethyl-9-phenyl-1,3,5,7-tetraazy-2,4,6,8,9-pentasily-[08.1^{1,5}]dicycle

Assemblies

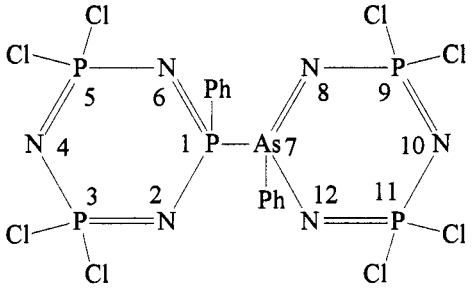
Examples:

1.



3,3,5,5,9,9,11,11-octachloro-1,7-diphenyl-2,4,6,8,10,12-hexaazy-1,3,5,7,9,11-hexaphosphy-[(06)1:7(06)]dicycle

The two modules are identical and thus either can act as a principal module. However, consider a case where P(7) is substituted by As:



2,4,6,8-tetraazy-1,3,5,7-tetrasulfy-[8]cycle
or
2,4,6,8-tetraazy-1,3,5,7-tetrasulfy-[08]cycle

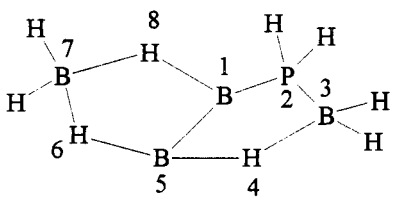
However, there is significant interaction between the sulfur atoms and therefore in some cases it might be preferable to name the compound as a cage instead of a simple monocycle.

2,4,6,8-tetraazy-1,3,5,7-tetrasulfy-[08.$0^{1,5}0^{3,7}$]tricycle

A particularly useful area of application for the nodal descriptor incorporated with the ring and chain nomenclature comprises the low-symmetry borane cages.

Examples:

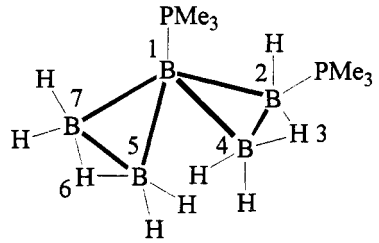
2.



2,2,3,3,7,7-hexahydrido-1,3,5,7-tetrabory-4,6,8-trihydrony-2-phosphy-[08.$0^{1,5}$]dicycle

Phosphorus is senior to hydrogen and thus establishes the direction of numbering of the main ring. While bridging hydrogen atoms could be named as bridging ligands, they can conveniently be incorporated in the nodal framework.

3.



2,4,4,5,5,7,7-heptahydrido-1,2-bis(trimethylphosphane)-1,2,4,5,7-pentabory-3,6-dihydrony-[04.3^{1,1}0^{2,4}0^{5,7}]tetracycle

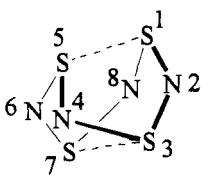
The nodal framework consists of two equivalent rings of four nodes. The main ring is selected by consideration of ligands (PMe_3 is senior to H).

The two modules differ only by their points of attachment. The principal module is determined according to the higher seniority of nitrogen to boron in the element seniority sequence.

Cage Compounds. The nodal descriptor establishes a connectivity, but not the geometry of the molecule. Most of the inorganic polycyclic compounds form cage structures. If the cage is relatively open and of low symmetry, it is advisable to use the present method involving nodal descriptors.

Example:

1.

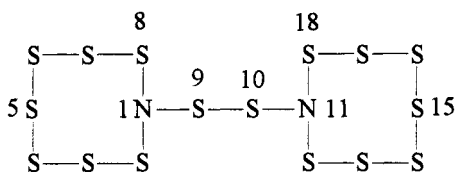


This molecule is often regarded as a simple monocyclic compound. Therefore it can be named as follows:

According to general nodal nomenclature (5) either ring can still constitute the principal module, but as phosphorus is senior to arsenic (1), it determines the numbering. The name is thus:

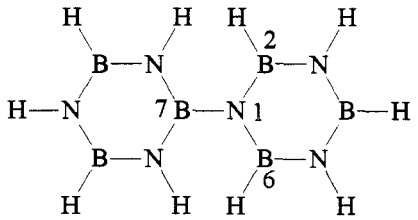
3,3,5,5,9,9,11,11-octachloro-1,7-diphenyl-7-arsy-2,4,6,8,10,12-hexaazy-1,3,5,9,11-penta-phosphy-[(06)1:7(06)]dicycle

2.



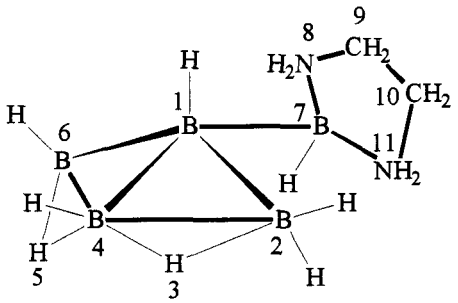
1,11-diazyhexadecasulfy-[(08)1:9(2)10:11(08)]catenadicycle

3.



2,3,4,5,6,8,9,10,11,12-decahydrido-1,3,5,8,10,12-hexaazy-2,4,6,7,9,11-hexabory-[(06)1:7(06)]dicycle

4.

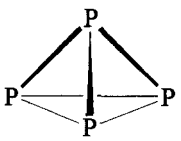


1,2,2,4,6,7,8,8,9,9,10,10,11,11-tetradecahydrido-8,11-diazy-1,2,4,6,7-pentabory-9,10-dicarby-3,5-dihydrony-[(06.$0^{1,4}0^{2,4}0^{4,6}$)1:7(05)]pentacycle

If the cage structure is of high symmetry, the description of the structure by the nodal descriptor is more problematic, since while it is possible to give a unique name to such a molecule, the visualization of the compound as a symmetric polyhedral cage is not easy.

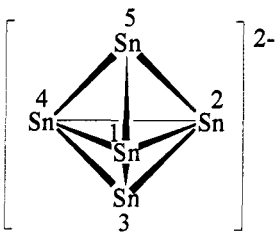
Examples:

5.



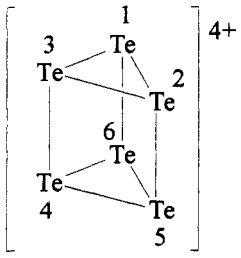
tetraphosphy-[04.$0^{1,3}0^{2,4}$]tricycle

6.



pentastanny-[05.$0^{1,3}0^{1,4}0^{2,4}0^{2,5}$]pentacyclate(2-) ion

7.



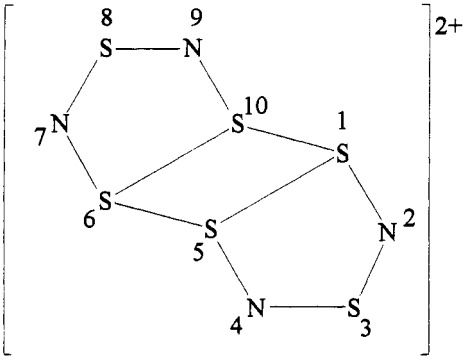
Hexatellury-[06.0^{1,3}0^{2,5}0^{4,6}]tetracyclium(4+) ion

In general, if the structure has a polyhedron of n faces, the compound will be named as a polycyclic entity consisting of n-1 rings. For most cases, however, high-symmetry cages are best named as clusters for which the nomenclature is presently being developed.

Ionic Species and Ligands. The names for the ions can conveniently be derived from the corresponding neutral molecules by modifying the names "catena" and "cycle". The charge number of the species is indicated in parentheses at the end of the name.

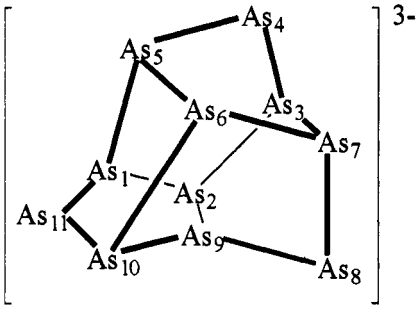
Examples:

1.



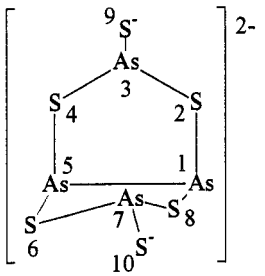
2,4,7,9-tetraazy-1,3,5,6,8,10-hexasulfy-[010.0^{1,5}0^{6,10}]tricyclium(2+) ion

2.



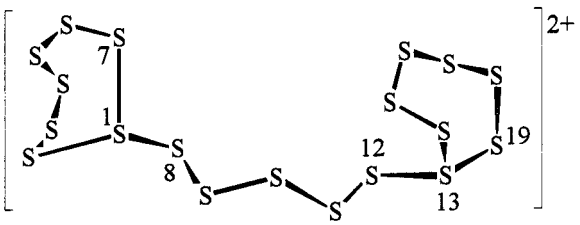
undecaarsy-[011.0^{1,5}0^{2,9}0^{3,7}0^{6,10}]pentacyclate(3-) ion

3.



3,7-disulfido-1,3,5,7-tetraarsy-2,4,6,8-tetrasulfy-[08.0^{1,5}]dicyclate(2-) ion

4.



nonadecasulfy-[(07)1:8(5)12:13(07)]catenadicyclium(2+) ion

When desirable, the location of the charge can be expressed by its nodal locant before the endings "-ium" or "-ate". The charges which are not located in the nodal framework cannot be indicated. Therefore, if the locations of the charges are needed, all pertinent atoms must be included in the nodal framework.

Example:

5. Consider the ion in example 3 of this section. To indicate the location of the charges the nodal skeleton must comprise two acyclic modules and one polycyclic module.

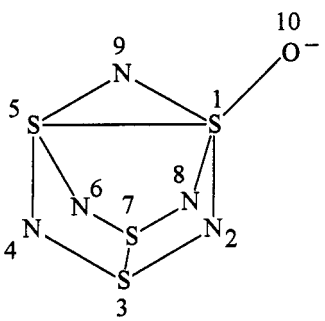
   1,3,5,7-tetraarsy-2,4,6,8,9,10-hexasulfy-[(08.0^{1,5})3:9(1)7:10(1)]dicatenadicycl-9,10-ate(2-) ion

   Note that the ending "-ate" does not imply that the cyclic module carries the charge. The locations of the charges are given unambiguously by the definitive nodal locants.

The construction of the ligand name follows the principles introduced in Chapter I-10 of "Nomenclature of Inorganic Chemistry" (1). The names of the cationic and neutral ligands are identical with the names of the free species, but the names of the anionic species are modified by replacing the ending "-ate" by the ending "-ato". The indicated donor atom must be a part of the nodal skeleton.

Examples:

6.

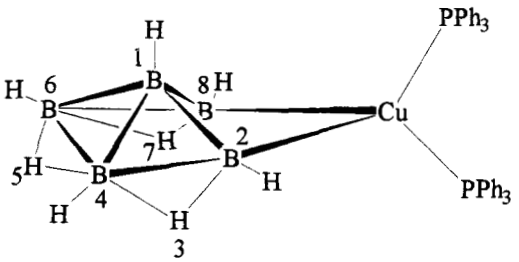


1-oxo-2,4,6,8,9-pentaazy-1,3,5,7-tetrasulfy-[08.1^{1,5}0^{1,5}0^{3,7}]tetracyclato

When the donor atom O(10) is indicated, the nodal skeleton must consist of two modules.

2,4,6,8,9-pentaazy-10-oxy-1,3,5,7-tetrasulfy-[(08.1^{1,5}0^{1,5}0^{3,7})1:10(1)]catenatetracycl-10-ato

7.



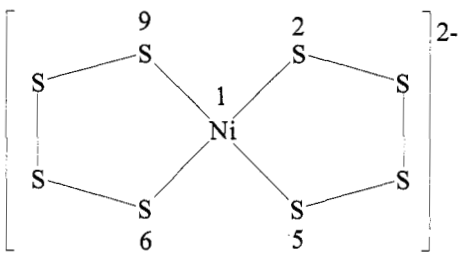
1,2,4,6,8-pentahydrido-1,2,4,6,8-pentabory-3,5,7-trihydrony-[08.0^{1,4}0^{1,6}0^{2,4}0^{4,6}0^{6,8}]hexacycl-2,8-atobis(triphenylphosphane)copper(I)

This compound can also be named as a coordination entity by considering the borane cage as a ligand.

Coordination Compounds. In certain cases it is preferable to name the complete coordination entity as a polycyclic compound. This approach is particularly useful for naming polynuclear complexes with purely inorganic chelating or bridging ligands.

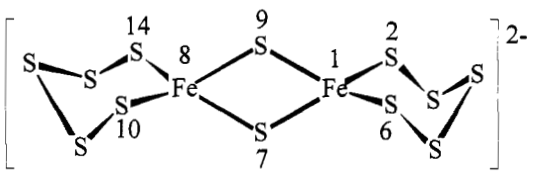
Examples:

1.



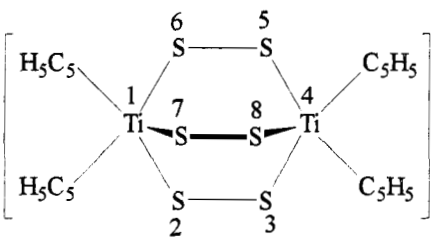
1-nickelyoctasulfy-[05.4^{1,1}]dicyclate(2-) ion

2.



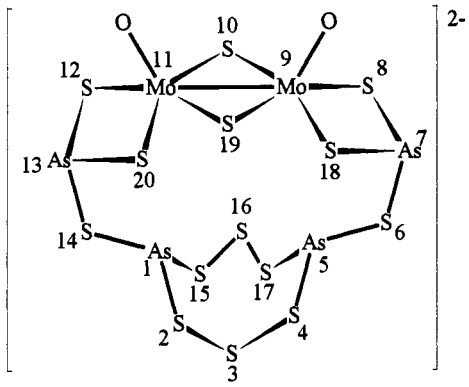
1,8-diferrydodecasulfy-[06.3^{1,1}5^{8,8}]tricyclate(2-) ion

3.



1,1,4,4-tetrakis(cyclopentadienyl)-1,4-dititany-2,3,5,6,7,8-hexasulfy-[06.2^{1,4}]dicycle

4.

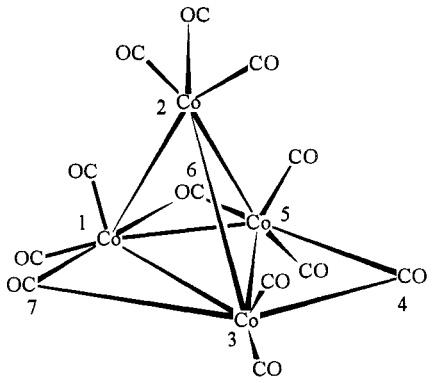


9,11-dioxo-1,5,7,13-tetraarsy-9,11-dimolybdytetradecasulfy-[014.3^{1,5}1^{7,9}1^{9,11}1^{11,13}0^{9,11}]hexacyclate(2-) ion

Polynuclear coordination compounds can also be treated as polycyclic compounds. It has to be kept in mind, however, that like in the case of non-metallic cage compounds the nodal descriptor does not give any indication of the geometry of the cluster; it only defines the connectivity. The nomenclature of cluster compounds is presently being developed by the the Commission on Nomenclature of Inorganic Chemistry.

Example:

5.



1,1,2,2,2,3,3,5,5-nonacarbonyl-4,6,7-trioxo-4,6,7-tricarby-1,2,3,5-tetracobalty-[06.1^{1,3}0^{1,3}0^{1,5}0^{2,5}0^{3,5}]hexacycle

FINAL REMARKS

This document presents a new additive method to name inorganic chain and ring compounds. Though it can be applied to any molecular species its use is mainly intended for compounds which are mainly or exclusively made up of atoms other than carbon. The application of the nodal descriptor enables the naming complicated polycyclic and branched chain compounds as well as compounds consisting of cyclic and acyclic modules. The selection of the nodal skeleton renders it possible to compare structurally analogous species regardless of their chemical identity.

The method is particularly suitable for low-symmetry ring and cage compounds and whenever it is important to establish the connectivity between the atoms. For high-symmetry cages and polynuclear coordination compounds the use of more exact structural descriptors is needed.

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