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Stereochemical Notation in Coordination Chemistry: Mononuclear Complexes of Coordination Numbers Seven, Eight, and Nine[1]

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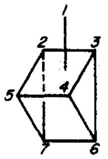
A unified system of notation for geometrical isomers is presented which includes central atom coordination symmetry and chirality for twelve coordination geometries of mononuclear complexes with coordination numbers 7, 8, and 9. The geometry of the central atom coordination sphere is given by a coordination system indicator, which consists of a two- or three-letter symmetry code and the coordination number of the central atom. The geometrical configuration is noted by a 7, 8, or 9 digit code consisting of the Cahn–Ingold–Prelog (CIP) priority rankings of the ligating atoms. The chirality of the central atom is determined by the unique progression of the CIP priority rankings of the ligating atoms and symbolized in the notation by the chirality symbols *C* (clockwise) and *A* (anticlockwise). This notation is consistent with and a direct extension of the stereochemical notation for mononuclear complexes of coordination numbers 4, 5, and 6 presented previously by the authors. It has been introduced into the Indexes to *Chemical Abstracts* starting with Volume 86 (January–June 1977).

Introduction

The stereochemistry of coordination compounds of the higher coordination numbers is generally described in the literature by the terms cis, trans; *fac*, *mer*; sym, asym; etc., or, more commonly, by a structure depicting the stereochemistry of the specific compound. Numbering systems[2,3] have also been developed for coordination polyhedra up to coordination number 20. However, such numbering systems have been noted to encounter certain serious difficulties.[4] The most notable problems with the above-mentioned terms and numbering systems can be shown by examining the structures illustrating the various isomers of the hypothetical monocapped trigonal-prismatic dichloropentafluoroniobate(2–) given in Figure 1.

There are five "cis" and three "trans" configurations for this compound, demonstrating that such binary terms are not sufficient to describe these eight structures. Numbering the chiral structures according to Muetterties and Wright[2] would yield the names listed in Table I. It is apparent from this list that a stereoisomer and its enantiomer cannot readily be distinguished by means of the Muetterties and Wright numbering system.

Table I. Chiral $[NbCl_2F_5]^{2-}$ Compounds



Muetterties-Wright Numbering

1,2-dichloro-3,4,5,6,7-pentafluoroniobate(2-)	I
1,3-dichloro-2,4,5,6,7-pentafluoroniobate(2-)	I
1,6-dichloro-2,3,4,5,7-pentafluoroniobate(2-)	VI
1,7-dichloro-2,3,4,5,6-pentafluoroniobate(2-)	VI
2,4-dichloro-1,3,5,6,7-pentafluoroniobate(2-)	VII
2,6-dichloro-1,3,4,5,7-pentafluoroniobate(2-)	VIII
2,7-dichloro-1,3,4,5,6-pentafluoroniobate(2-)	IV
3,5-dichloro-1,2,4,6,7-pentafluoroniobate(2-)	VII
3,6-dichloro-1,2,4,5,7-pentafluoroniobate(2-)	IV
3,7-dichloro-1,2,4,5,6-pentafluoroniobate(2-)	VIII

Another problem inherent in the use of fixed numbering to distinguish isomers of coordination polyhedra is illustrated by the hypothetical structure in Figure 2. This structure may be named either 3-ammine-1,5;2,6;4,7-tris(2-aminoethanolato-*O*,*N*)niobium[5] or 5-ammine-1,3;2,6;4,7-tris(2-aminoethanolato-*O*,*N*)niobium. A set of priorities for the ligating atoms is needed for a numbering system to be definitive, particularly for unsymmetrical and more complicated chelating structures. It has recently been noted by Ruch that regardless "of the relevance of classification" there is a need for a nomenclature to distinguish isomers.[6]

In a paper previously published in this journal,[7] we described a notation utilizing the Cahn–Ingold–Prelog (CIP) standard sequence rule[8] to rank ligating atoms and thus provide a notation for completely describing the stereochemistry of the six prevalent central-atom geometries of mononuclear complexes of coordination numbers 4, 5, and 6. We now extend the notation to completely describe the stereochemistry of the twelve prevalent geometries for the central atoms in mononuclear complexes of coordination numbers 7, 8, and 9. This notation has been introduced into the Indexes to *Chemical Abstracts* for the Tenth Collective Period (1977–1981).

Principles

The stereochemical descriptors for mononuclear compounds of the higher coordination numbers are comprised of four parts: (a) a symmetry site term, (b) a configuration number, (c) a chirality symbol, and (d) a ligand stereochemical segment.

Symmetry Site Term. The symmetry site term for the higher coordination geometries consists of a two- or three-letter code expressing the idealized molecular geometry about the central atom and the coordination number of the central atom. These symmetry site terms are derived directly from commonly used descriptive geometric terms. Although distortions from idealized geometry occur widely in nature, the commonly used practice of relating molecular structures to idealized models appears to be a practical principle on which to base a qualitative notation. The twelve symmetry site terms for polyhedra of coordination numbers 7, 8, and 9 are given in Table II.

Configuration Number. The configuration number for the higher ligancy complexes is a 7, 8, or 9 digit numerical designation of the CIP priority numbers for all ligating atoms in the structure. The configuration number distinguishes between the various geometric isomers. The CIP relative priority numbers for ligating atoms are determined according to the subrules of the CIP sequence rules[8] which, stated briefly, are (1) higher atomic number precedes lower, (2) higher atomic mass number precedes lower, (3) *Z* precedes *E*,[9] (4) like pair *R*,*R* or *S*,*S* precedes unlike pair *R*,*S* or *S*,*R*, and (5) *R* precedes *S*.

The same relative priority numbers are assigned to all constitutionally equivalent atoms. For example, in the system $Ma_2b_3c_2$, where M is a central atom and a, b, and c represent monodentate ligands, the relative priority numbers are 1,1,2,2,2,3,3. The twelve model polyhedra for coordination numbers 7, 8, and 9 are of lower symmetry than an octahedron. Preference between equivalent ligating atoms is determined, first, by considering the symmetry elements of the specific

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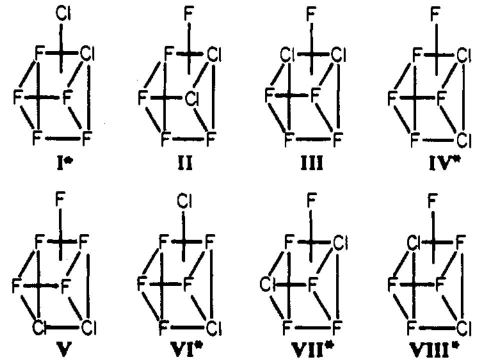


Figure 1. Isomers of $[NbCl_2F_5]^{2-}$ (chiral structures are indicated by an asterisk).

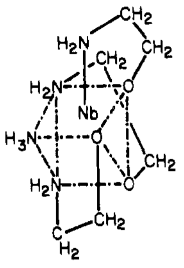


Figure 2. $[Nb(C_2H_6NO)_3(NH_3)]$.

polyhedra and, second, by citing the CIP priority numbers in order to give the lowest numerical sequence; e.g., 11325 is a lower sequence than 11352.[10]

When there are two or more equivalent bidentate or tridentate ligands in the same system, and thus, the same priority numbers are established in equivalent ligands, the ties are broken by identically priming all the CIP priority numbers of the ligating atoms within each ligand to uniquely determine both the configuration number and the chirality label. In complexes with symmetrical polydentate ligands, i.e., tetradentate, hexadentate, etc. (including symmetrical macrocyclic ligands), ties between equivalent ligating atoms are broken by priming the ligating atom priority numbers in chelating groups or pairs, thus reducing a polydentate ligand to groupings of equivalent bidentate or tridentate ligands. When two or more nonequivalent tie-breaking choices exist for the polyhedra of coordination numbers 7, 8, and 9, the tie is resolved, first, by assigning the lowest priming value to atom priority numbers at positions on the preferred symmetry axis or plane and, second, by assigning the priming so that the lowest ordered numerical sequence for the configuration number is obtained at the first point of difference. All priming is cited in the configuration number.[11]

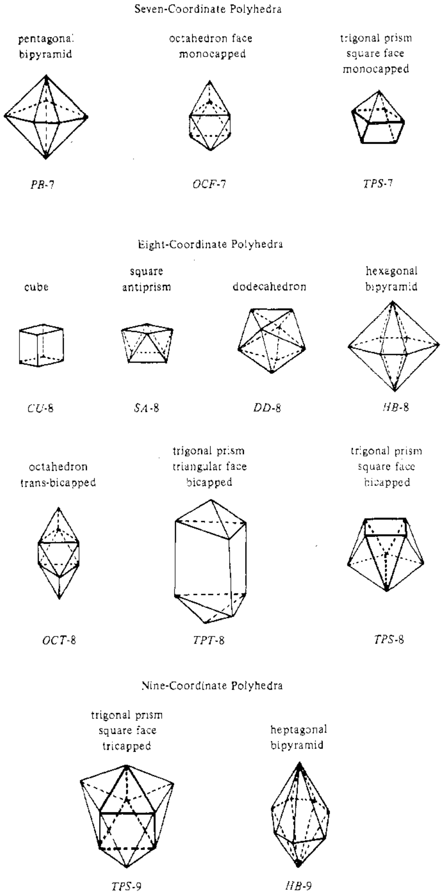
Chirality Symbol. The chirality symbols *C* (clockwise or right-handed) and *A* (anticlockwise or left-handed[12]) are used to denote the absolute stereochemistry in all twelve polyhedra for the higher coordination numbers.

Ligand Stereochemical Segment. The ligand stereochemical segment, except for stereoparents,[13] is set off in enclosing marks and cited after the central metal atom stereonotation; e.g., see (R^*,R^*) in Figure 5. When it is necessary to associate a locant with the ligand stereonotation to avoid ambiguity, the CIP priority number of the ligating atom is used as the locant. The lowest CIP priority number is used for polydentate ligands. Stereodescriptors for stereoparents are cited in the ligand portion of the compound name.

Assignment of Configuration Numbers

The configuration number is assigned by orienting the model structure with the highest-order axis in the vertical plane. The model structure is then viewed from the highest CIP priority ligating atom on the highest-order axis or from a point on the highest-order axis above the most preferred end or terminal plane perpendicular to the axis. The most preferred end or terminal plane is that end plane which either contains the greatest number of atoms, contains the greatest number of highest CIP priority ligating atoms, or is adjacent to a plane containing the greatest number of highest CIP priority ligating atoms. Note that the *OCF*-7 (octahedron face monocapped), *TPS*-7 (trigonal prism square face monocapped), and *TPS*-8 (trigonal prism square face bicapped) model structures are of low symmetry and have only one correct orientation.

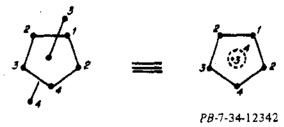
Table II. Symmetry Site Terms



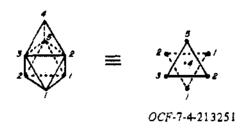
The configuration numbers for the model structures coded *PB*-7, *OCF*-7, *TPS*-7, *HB*-8, *OCT*-8, *TPT*-8, and *HB*-9 begin with the CIP priority numbers of the ligating atom(s) on the highest-order axis and are given in lowest numerical order sequence; see Table II above. These priority numbers for atoms on the highest-order axis are separated from the remainder of the configuration number by a hyphen, e.g., *PB*-7-XX-XXXXX or *OCF*-7-X-XXXXXX. The remaining portion of the configuration number for these seven model structures is derived by viewing the structure from the highest CIP priority ligating atom on the highest-order axis, or from the axial ligating atom located above the preferred plane, and by citing the CIP priority number of the ligating atom with the highest CIP priority in the plane adjacent to that atom. The configuration number is then completed by continuing to cite the CIP priority numbers of the ligating atoms in sequence as they are encountered, either clockwise or anticlockwise around the projection of the model structure, alternating between planes, where necessary. For those model structures with eclipsed pairs of ligating atoms, the CIP priority numbers are given in pairs with the priority number for the preferred atom in the first plane followed by the priority number for the ligating atom it eclipses. The remaining ligating atom CIP priority numbers are given as they are

Table III. Derivation of Configuration Numbers for Twelve Model Polyhedra

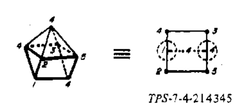
1. Pentagonal bipyramid



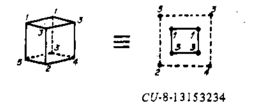
2. Octahedron face monocapped



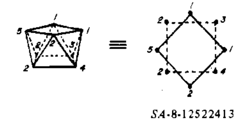
3. Trigonal prism square face monocapped



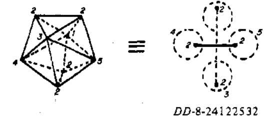
4. Cube



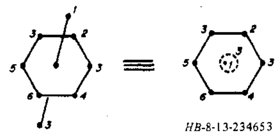
5. Square antiprism



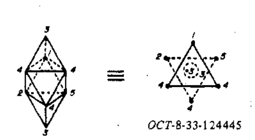
6. Dodecahedron



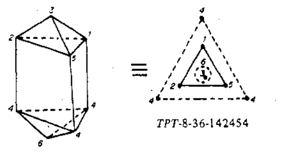
7. Hexagonal bipyramid



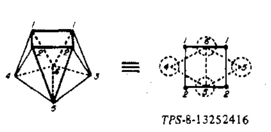
8. Octahedron trans-bicapped



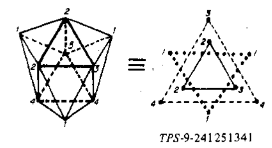
9. Trigonal prism triangular face bicapped



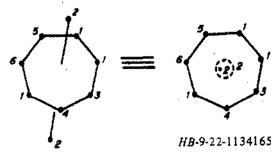
10. Trigonal prism square face bicapped



11. Trigonal prism square face tricapped



12. Heptagonal bipyramid

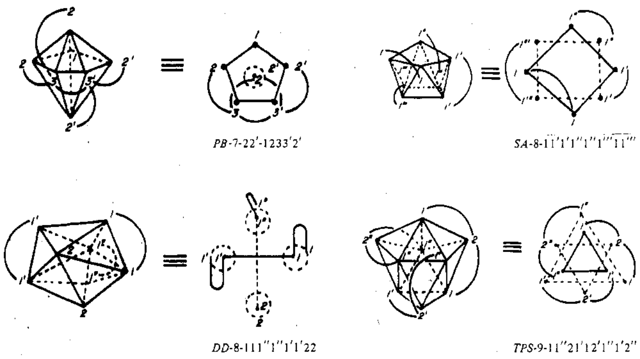


encountered, either clockwise or anticlockwise around the projection of the model structure as viewed from the preferred end of the highest-order axis. For compounds in which a clockwise or anticlockwise citation of the configuration number gives two different configuration numbers (generally chiral compounds), the correct one is the lowest numerical sequence determined at the first point of difference.

The remaining five model structures, *CU*-8, *SA*-8, *DD*-8, *TPS*-8, and *TPS*-9, do not have a ligating atom on the highest-order axis and, thus, do not have a distinct portion of the configuration number separated by a hyphen. These model structures are viewed from a point on the highest-order symmetry axis above the preferred terminal plane as defined previously. The configuration number is derived by first citing the CIP priority number of the preferred ligating atom in the preferred end plane and then citing the CIP priority number of the ligating atom it eclipses, if one exists. In the next step, one proceeds clockwise or anticlockwise around the projection of the model structure, giving the priority numbers of the ligating atoms as they are encountered, alternating between planes when necessary. Again, the clockwise or anticlockwise direction is chosen to give the lowest-order numerical sequence for the configuration number determined at the first point of difference. The derivation of the configuration number for twelve model polyhedra is illustrated in Table III.

The assignment of the configuration number for complexes with chelating ligands follows the same procedures except that primed priority numbers must be employed to remove the degeneracy of equivalent donor atoms in identical bidentate and tridentate ligands and in the equivalent groupings of symmetrical polydentate chelating ligands. The derivation of configuration numbers for chelating ligands is illustrated in Table IV.

Table IV. Derivation of Configuration Numbers for Chelated Structures



Assignment of Chirality Labels

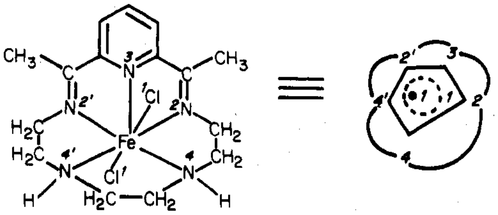
The chirality labels *C* and *A* are assigned to distinguish enantiomers for all the higher coordinate polyhedra. The chirality labels are assigned by viewing the model structure from the highest CIP priority ligating atom on the highest-order axis of the structure or by viewing the model structure from above the preferred terminal plane. Accordingly, the chiral structure is given the label *C* or *A*, depending upon whether the sequence of the CIP priority numbers indicates a clockwise or anticlockwise direction.

Assignment of Stereochemical Notation

A. Seven-Coordination. 1. Pentagonal Bipyramid (*PB*-7). The symmetry site code *PB* and coordination number 7 are assigned to the iron complex shown in Figure 3. The ligating atom priority numbers are assigned as follows: the chlorine atoms have the highest atomic number (17) and are given the relative priority number 1. An exploration table is prepared for the nitrogen atoms of the macrocyclic ring; see Table V. The relative priority numbers are assigned by inspecting the exploration table: 2 for the imino ring nitrogen, 3 for the pyridine ring nitrogen, and 4 for the secondary amine ring nitrogen.

The configuration number starts with the CIP priority numbers of the ligating atoms on the C_5 axis in lowest numerical sequence, i.e., 11. The pentagonal plane is viewed from the atom of highest CIP priority (lowest priority number) on the axis. The remaining portion of the configuration number, set off by a hyphen, is given by starting with the highest CIP priority atom in the plane, and then by proceeding either right or left, to give the lowest numerical sequence of numbers (the series 232'4'4 < 244'2'3). When the structure is chiral, the chiral label *C* or *A* is assigned as described above.

2. Octahedron Face Monocapped (*OCF*-7). For the molybdenum compound shown in Figure 4, the symmetry site

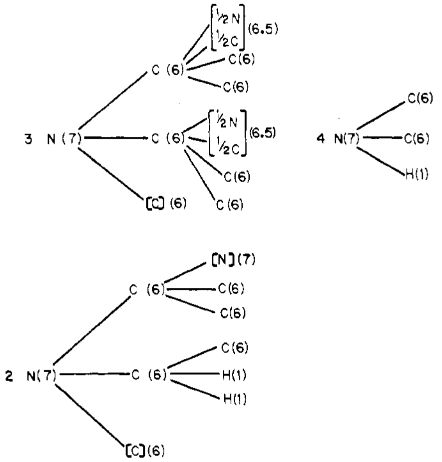


Configuration number = 11-232'4'4
Chirality = none

(PB-7-11-232'4'4)-dichloro(2,13-dimethyl-3,6,9,12,18-pentaazabicyclo[12.3.1]octadeca-1(18),2,12,14,16-pentaene-N^3,N^6,N^9,N^{12},N^{18})iron(1+)

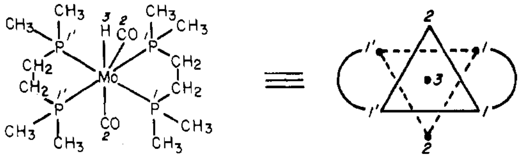
Figure 3. $[Fe(C_{15}H_{23}N_5)Cl_2]^+$.

Table V. Exploration Table for Macrocyclic Ring from Figure 3



code *OCF* and coordination number 7 are assigned. The configuration number begins with the CIP priority number of the ligating atom on the C_3 axis. The structure is viewed from this position and the highest CIP priority (lowest number) atom in the adjacent plane is given next in sequence after a hyphen. The next number is obtained by proceeding right or left in the second plane to the highest CIP priority atom adjacent to the position of the preferred ligating atom in the first plane of the structure. The remaining numbers of the configuration number are derived by citing the CIP priority numbers of the atoms as they are encountered, proceeding in the same direction, alternating from the first to the second plane and back around the structure. For chiral compounds, the chirality labels are assigned as stated above.

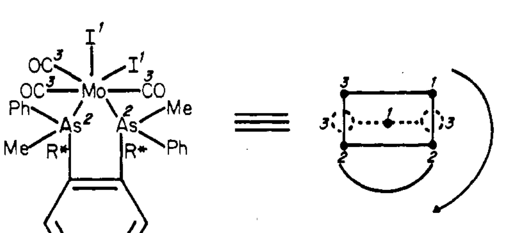
3. Trigonal Prism Square Face Monocapped (*TPS*-7). The symmetry site code *TPS* and the coordination number 7 are assigned to the molybdenum compound shown in Figure 5. The first digit of the configuration number is the CIP priority number of the donor atom on the C_2 axis. The structure is viewed from the donor atom on the C_2 axis, and the CIP priority number of the highest priority donor atom in the adjacent plane is then given after a hyphen. The next digit is the priority number of the nearest-neighboring atom, right or left, in the next or last plane of the structure. This establishes the direction, either right or left, around the model structure, and the remaining priority numbers of the configuration number are cited as they are encountered, continuing in this direction around the projection of the model structure. Chirality labels are assigned as stated previously.



Configuration number = 3-1121'1'2
Chirality = none

(*OCF*-7-3-1121'1'2)-dicarbonylbis[1,2-ethanediylbis[dimethyl=phosphine]-*P*,*P'*]hydromolybdenum(1+)

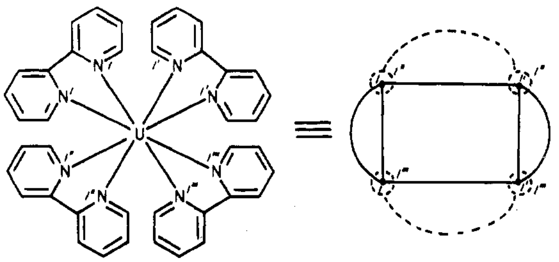
Figure 4. $[Mo(CO)_2(C_6H_{16}P_2)_2H]^+$.



Configuration number = 1-132233
Chirality = *C*

[*TPS*-7-1-132233-*C*-(*R**,*R**)]-tricarbonyldiiodo[1,2-phenyl=enebis[methylphenylarsine]-*As*,*As'*]molybdenum

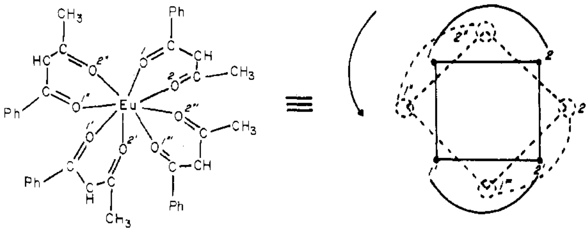
Figure 5. $[Mo(CO)_3I_2(C_{20}H_{20}As_2)]$.



Configuration number = 11''11'''1'1'''1'1''
Chirality = none

(*CU*-8-11''11'''1'1'''1'1'')-tetrakis(2,2'-bipyridine-*N*,*N'*)=uranium

Figure 6. $[U(C_{10}H_8N_2)_4]$.



Configuration number = 11''1'1'''2'2'''22''
Chirality = *A*

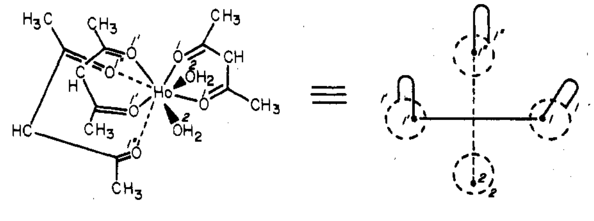
(*SA*-8-11''1'1'''2'2'''22''-*A*)-tetrakis(1-phenyl-1,3-butanedionato-=*O*,*O'*)europate(1-)

Figure 7. $[Eu(C_{10}H_9O_2)_4]^-$.

B. Eight-Coordination. 1. Cube (*CU*-8). The eight-coordinate uranium compound in Figure 6 is assigned the symmetry site code *CU* and coordination number 8. The configuration number is assigned by viewing the structure from a point on the C_4 axis above the preferred face (that face which contains the greatest number of highest CIP priority ligating atoms). The priority number of the highest priority atom in the preferred face is given, followed by the priority number of the donor atom it eclipses. The priority number of the next donor atom is assigned by proceeding either right or left in the preferred plane to the neighboring atom of highest priority. This priority number is followed by the priority number for the donor atom it eclipses. The remainder of the configuration number is derived by continuing around the structure in a like sequence. Chirality labels are assigned to chiral structures as stated above.

2. Square Antiprism (*SA*-8). For the europium compound given below in Figure 7, the symmetry site code *SA* and coordination number 8 are assigned. The configuration number is assigned by viewing this structure from a point on the C_4 axis above the preferred face and citing first the priority number of the highest priority atom in this face. The second integer in the configuration number is determined by proceeding either right or left to the highest priority donor atom occupying an adjacent position in the second plane. Then the priority numbers of the ligating atoms are given as they are encountered, by continuing in the same direction and by alternating between planes around the projection of the structure. Again, chirality labels are assigned when appropriate.

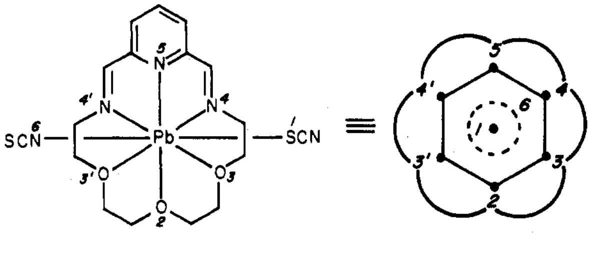
3. Dodecahedron (*DD*-8). The symmetry code *DD* and coordination number 8 are assigned to the holmium compound



Configuration number = 111″1″1′1′22
Chirality = none

(*DD*-8-111″1″1′1′22)-diaquatris(2,4-pentanedionato-*O*,*O*′)=holmium

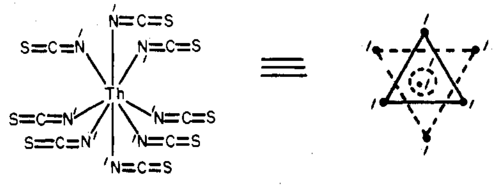
Figure 8. $[Ho(H_2O)_2(C_5H_7O_2)_3]$.



Configuration number = 16-23454′3′
Chirality = none

(*HB*-8-16-23454′3′)-(thiocyanato-*N*)(thiocyanato-*S*)(3,15,21-triaza-=6,9,12-trioxabicyclo[15.3.1]heneicosa-1(21),2,15,17,19-pentaene-=N^3,N^{15},N^{21},O^6,O^9,O^{12})lead

Figure 9. $[Pb(NCS)(SCN)(C_{15}H_{21}N_3O_3)]$.



Configuration number = 11-111111
Chirality = none

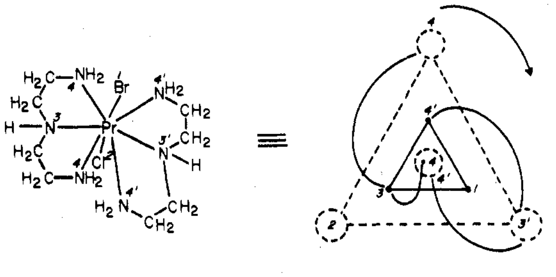
(*OCT*-8-11-111111)-octakis(thiocyanato-*N*)thorate(4-)

Figure 10. $[Th(NCS)_8]^{4-}$.

illustrated in Figure 8. The structure is viewed from a point on the C_2 axis above the preferred terminal plane (edge). The configuration number is assigned by citing the priority number of the highest priority ligating atom in the first plane (edge), followed by the priority number of the atom in the third plane that is eclipsed or partially eclipsed by this atom. Then its priority number is given by proceeding right or left to the highest priority atom in the second plane. This priority number is followed by that of the eclipsed donor atom in the fourth plane (edge). As one continues in the same direction, the priority numbers of donor atom and eclipsed donor atom partners are given as they are encountered. Chirality labels *C* or *A* are assigned when appropriate.

4. Hexagonal Bipyramid (*HB*-8). For the lead compound shown in Figure 9, the symmetry site code *HB* and coordination number 8 are assigned. The configuration number is assigned in the same way as that of the pentagonal bipyramid (*PB*-7) above. For chiral structures, the chirality labels are assigned in the same manner as given above.

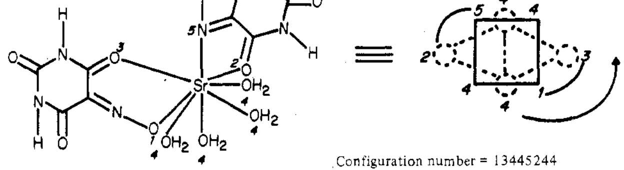
5. Octahedron Trans-Bicapped (*OCT*-8). The thorium compound in Figure 10 is assigned the symmetry site code *OCT* and the coordination number 8. The configuration number for this structure starts with the CIP priority numbers for the donor atoms on the C_3 axis cited in lowest numerical sequence and is separated by a hyphen from the remaining six priority numbers. The rest of the configuration number is derived in the same manner as that of the octahedron face monocapped structure (*OCF*-7) above. The chirality labels are also assigned as stated previously.



Configuration number = 44′-13′324′4
Chirality = *C*

(*TPT*-8-44′-13′324′4-*C*)-bis[*N*-(2-aminoethyl)-1,2-ethanediamine-=*N*,*N*′,*N*″]bromochloropraseodymium(1+)

Figure 11. $[Pr(C_4H_{13}N_3)_2BrCl]^+$.



Configuration number = 13445244
Chirality = *A*

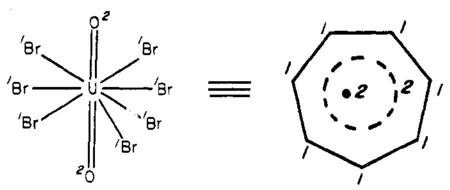
(*TPS*-8-13445244-*A*)-tetraaqua(2,4,5,6(1*H*,3*H*)-pyrimidinetetrone 5-=oximato-N^5,O^4)(2,4,5,6(1*H*,3*H*)-pyrimidinetetrone 5-oximato-O^4,O^5)=strontium

Figure 12. $[Sr(H_2O)_4(C_4H_2N_3O_4)_2]$.

6. Trigonal Prism Triangular Face Bicapped (*TPT*-8). The symmetry site code *TPT* and coordination number 8 are assigned to the praseodymium compound in Figure 11. The configuration number for this structure begins with the priority numbers for the donor atoms on the C_3 axis, given in lowest numerical sequence and set off by a hyphen from the remaining six priority numbers. The structure is viewed from the highest priority donor atom on the C_3 axis or the donor atom on the C_3 axis above the preferred plane. The priority number for the highest priority atom in the adjacent plane is cited next in the configuration number, along with the priority number for the donor atom it eclipses. As one proceeds either right or left to the donor atom of next highest priority in the upper plane, this atom's CIP priority number, along with the priority number of the atom it eclipses, is given. The final two numbers of the configuration number are given in a like sequence. Chirality labels are assigned when appropriate.

7. Trigonal Prism Square Face Bicapped (*TPS*-8). For the strontium compound given in Figure 12, the symmetry site code *TPS* and coordination number 8 are assigned. The configuration number is assigned by viewing the structure from a point on the C_2 axis above the uncapped square or rectangular face. The first digit of the configuration number is the priority number of the highest CIP priority atom in the square face. The next priority number cited is that of the adjacent atom encountered as one proceeds either right or left to the atom in the plane adjacent to the square face. As one continues in the same direction, the priority numbers for the ligating atoms are given as they are encountered when one views the projection of the structure from the C_2 axis above the square face. When a choice exists to proceed either right or left from the first donor atom cited in the configuration number, the choice is determined by giving the lowest numerical sequence to the configuration number at the first point of difference. Chirality labels are assigned as described previously.

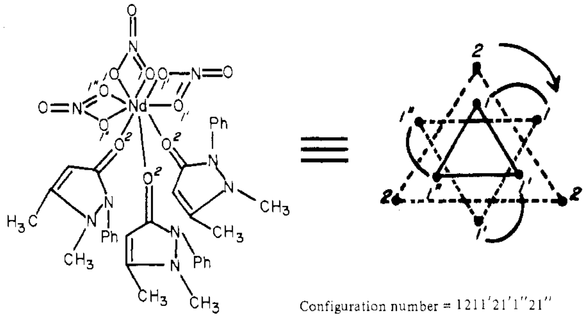
C. Nine-Coordination. 1. Heptagonal Bipyramid (*HB*-9). The symmetry site code *HB* and coordination number 9 are



Configuration number = 22-1111111
Chirality = none

(*HB*-9-22-1111111)-heptabromodioxouranate(5-)

Figure 13. $[UBr_7O_2]^{5-}$.



Configuration number = 1211′21′1″21″
Chirality = *C*

(*TPS*-9-1211′21′1″21″-*C*)-tris(1,2-dihydro-1,5-dimethyl-2-phenyl-3*H*-pyrazol-3-one-*O*)tris(nitrato-*O*,*O*′)neodymium

Figure 14. $[Nd(C_{11}H_{12}N_2O)_3(NO_3)_3]$.

assigned for the uranium compound in Figure 13. The configuration number is assigned in the same way as that of the pentagonal bipyramid (*PB*-7) structure above and chirality labels are also assigned as stated above.

2. Trigonal Prism Square Face Tricapped (*TPS*-9). For the neodymium compound illustrated in Figure 14, the symmetry site code *TPS* and coordination number 9 are assigned. The configuration number is assigned by viewing the structure from a point on the C_3 axis above the preferred end plane. The configuration number begins with the CIP priority number for the most preferred donor atom in the preferred end plane cited with the priority number of the atom it eclipses. Then as one proceeds either right or left to the adjacent most preferred donor atom in the middle plane, its priority number is given next in sequence. By continuing in the same direction and returning to the preferred end plane, one cites the priority numbers of the next donor atom and its eclipsed partner. The remainder of the configuration number is derived in the same manner. Chirality labels are assigned to chiral structures as stated above.

Conclusion

The stereochemical notation introduced in the Indexes to *Chemical Abstracts* for the Tenth Collective Period (1977–1981) for mononuclear complexes of coordination numbers 7, 8, and 9, representing twelve geometries, has been presented with illustrative examples. This notation is a direct extension of the notation described in an earlier report and is compatible with the other stereochemical notations used by Chemical Abstracts Service in its computer processing of chemical information. As further need arises in ongoing processing, notation for new geometries and higher coordination numbers will be added to the stereochemical notation system for mononuclear complexes. The new symmetry site codes and configurational notation will be reported in the next Index Guide or its supplement.

The evaluation of present and future proposals for extending the stereochemical notation to coordination numbers higher than 4 in organic ring compounds and polynuclear complexes will continue. The goal of this evaluation will be to give specific, unique notations for these compounds in the information systems of Chemical Abstracts Service and the indexes to *Chemical Abstracts*.

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References and Notes

(1) This work was presented in part at the 172nd National Meeting of the American Chemical Society, San Francisco, Calif., Aug 29–Sept 3, 1976, by M. F. Brown, B. R. Cook, and T. E. Sloan: Paper 228, Division of Inorganic Chemistry.
(2) E. L. Muetterties and C. M. Wright, *Q. Rev., Chem. Soc.*, **21** (1), 109–194 (1967).
(3) "IUPAC Nomenclature of Inorganic Chemistry", 2nd ed, Butterworths, London, 1971, Rule 7.5.
(4) For a comprehensive discussion of numbering systems for describing coordination polyhedra, see M. F. Brown's Master's Thesis, The Ohio State University, 1970.
(5) Rule 7.513, "IUPAC Nomenclature of Inorganic Chemistry 1970", states "Difference in end groups which can coordinate: the end with the element which occurs earlier in the series in Table IV" gives the order O, N for the coordination ligand locant. *Chemical Abstracts* index nomenclature gives the symbols for the coordination ligand locant in alphabetical order.
(6) E. Ruch, *Angew Chem., Int. Ed. Engl.*, **16**, 65–72 (1977).
(7) M. F. Brown, B. R. Cook, and T. E. Sloan, *Inorg. Chem.*, **14**, 1273–1278 (1975).
(8) R. S. Cahn, C. Ingold, and V. Prelog, *Angew Chem., Int. Ed. Engl.*, **5**, 385 (1966); *J. Org. Chem.*, **35**, 2849 (1970).
(9) In ref 8, this is given as "seqcis precedes seqtrans". For the definition of *E* and *Z* see J. E. Blackwood, C. L. Gladys, K. L. Loening, A. E. Petrarca, and J. E. Rush, *J. Am. Chem. Soc.*, **96**, 1748 (1974).
(10) For a further discussion of lowest sequence in numbering, see "IUPAC Nomenclature of Organic Chemistry", Section A, Butterworths, London, 1971, Rule 2.2.
(11) Priming is only given in the configuration number for the *lower* coordination numbers in the cases of the six-coordinate octahedra with two identical symmetrical tridentate ligands and the six-coordinate trigonal prism.
(12) We have selected the less common term "anticlockwise" in preference to "counterclockwise" in order to provide a mnemonic for the second chirality label, i.e., *A*.
(13) J. E. Blackwood, P. M. Elliott, R. E. Stobaugh, and C. E. Watson, *J. Chem. Inf. Comput. Sci.*, **17**, 3–8 (1977).