

clature, which would be for all intents and purposes thoroughly systematic, is real, and the accomplishment of such an objective is not to be ruled out. Such a systematic nomenclature would retain as much as possible of present organic rules and principles and would add new rules only where present rules are inadequate or overcomplex. Admittedly, it would lead to many names strange to us, but it would have the advantages of maximum simplicity of rules and minimum burden on memory, particularly for chemists of coming generations. The technical feasibility of developing a thoroughly systematic syllabic organic nomenclature by reconstructing established rules and adding new rules where needed was demonstrated by the proposals of Dyson (4) and Taylor (5) and by extensive experimentation at the American Cyanamid Co. a number of years ago. However, among the questions which must be answered before official work along these lines by the American Chemical Society or by IUPAC can be justified are: (1) Would an extensively modified systematic nomenclature be considered for adoption by *Chemical Abstracts*? and (2) What would be its chances for eventual use by chemists in reports and publications? Attempts to answer these questions will provide the basis for much discussion and debate by the many parties involved, when and if

serious consideration is given to the development and introduction of a fully systematic organic nomenclature.

LITERATURE CITED

- (1) International Union of Pure and Applied Chemistry, Nomenclature of Organic Chemistry, Definitive Rules for Section A. Hydrocarbons, Section B. Fundamental Heterocyclic Systems, London, Butterworths, 1958; *J. Am. Chem. Soc.* **82**, 5545-74 (1960).
- (2) International Union of Pure and Applied Chemistry, Nomenclature of Organic Chemistry, Definitive Rules for Section C. Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium, London, Butterworths, 1965.
- (3) Patterson, A. M., Definitive Report of the Commission on the Reform of the Nomenclature of Organic Chemistry (Translation with Comments), *J. Am. Chem. Soc.*, **55**, 3905-25 (1933).
- (4) Dyson, G. M., *A New Notation for Organic Chemistry*. Royal Institute of Chemistry Lecture, published jointly with the Chemical Society and the Society of Chemical Industry, 1946; Dyson, G. M., "A New Notation and Enumeration System for Organic Compounds," Longmans, London, 1947; 2nd ed., 1949. Dyson, G. M., *Research (London)* **2**, 104-15 (1949).
- (5) Taylor, F. L., *Ind. Eng. Chem.* **40**, 734-8 (1948).

Inorganic Nomenclature in 1966: Progress and Problems*

ROY M. ADAMS†
Geneva College, Beaver Falls, Pennsylvania

Received March 24, 1966

A brief discussion of the history and current status of inorganic nomenclature is presented along with a discussion of the relationship between the American Chemical Society's work in inorganic nomenclature and that of the International Union of Pure and Applied Chemistry. Problem areas, especially those in the nomenclature of boron compounds, inorganic polymers, and cluster compounds are discussed.

The standardization of nomenclature practice is always a slow and halting process. Different workers in the same country have different nomenclature needs arising from different approaches to the same problem; in particular, workers from different language backgrounds have an increased problem in finding a uniformly acceptable nomenclature. The first definitive report of the Inorganic Nomenclature Commission of the International Union for Pure and Applied Chemistry (IUPAC) appeared in 1940

(1) and the second in 1957 (2). Currently the commission is taking steps to update and strengthen the 1957 report with a view toward publication of a tentative report in 1967 and a new definitive report in 1968. Since coordination nomenclature seems to be capable of unifying nearly all types of inorganic nomenclature, changes which appear to the writer to be most significant are in this area and include:

1. adoption of alphabetical order for ligands;
2. acceptance of the Ewens and Bassett system as an alternate to Stock numbers;
3. acceptance of the McDonnell and Pasternack system for designation of stereoisomerism.

* Presented before the Division of Chemical Literature, Symposium on Chemical Nomenclature, 152nd National Meeting of the American Chemical Society, New York, N. Y., Sept. 15, 1966.

† Chairman, Nomenclature Committee, Division of Inorganic Chemistry, American Chemical Society.

Alphabetical order for ligands replaces the 1957 rule (7.25), presently also being followed by *Chemical Abstracts* (3), which listed ligands in the order anionic > neutral > cationic, with a complex order of precedence within these classes. This new recommendation follows the practice which was recommended in the American version of the 1957 report and is used by *Chemical Abstracts* in 1967. However, it goes farther in removing all classification on the basis of charge type. There are some inorganic chemists who would favor alphabetical order within the above classes with a reversal of the priority of the classes. This would presumably remove confusion as to whether an anionic ligand was attached to the central atom or to a neutral ligand—e.g., ethylenetrichloroplatinum(II) is clearer orally than trichloro(ethylene)platinum. However, the present decision is to use straight alphabetical order throughout with liberal use of parentheses to avoid confusion in written practice. In oral practice it would appear wise to allow any order necessary to make clear distinctions.

The Ewens and Bassett system (4) uses as a suffix the charge of the complex in Arabic numerals enclosed in parentheses instead of the Stock number (oxidation state). This provides a number which most chemists would agree is real, rather than an arbitrary designation such as the oxidation state—e.g., $\text{CoCl}_4(\text{NH}_3)_2^{1-}$ may be named diamminetetrachlorocobaltate(1-) or diamminetetrachlorocobaltate(III). The great advantage comes in polynuclear complexes where oxidation states are mixed or fractional. B_3H_8^- as octahydrotriborate(1-) is much more satisfactory than octahydrotriborate(II, II, III). This also makes considerably more feasible the use of the same name for the same group whether present as an inorganic ligand or as an organic substituent—i.e., the “-o” suffix to indicate anionic character is less necessary. This may lead to bridging different practices in these areas (2).

The McDonnell and Pasternack system (5) for designation of stereoisomerism chooses the major symmetry axis of the coordination polyhedron. Since numbers have generally been used for locating the different atoms in a chain, it was felt best to use letters to designate different positions in the coordination sphere (6). As one proceeds down this axis, the first coordinated atom or plane of atoms encountered is lettered alphabetically in a clockwise fashion. Then in proceeding to the next plane, a finite clockwise rotation from the last atom lettered is made to determine the first atom to be lettered in that plane. In other words, the major symmetry axis is viewed as a right-handed screw axis. For equivalent positions the ligand with alphabetical priority is lettered first. This leads to the designation shown in Figures 1 and 2 for octahedral coordination, which is at present of greatest importance in complex metal stereoisomerism. Rules have also been prepared to cover orders of numbering for chelating ligands and those with branching. Copies may be obtained from Dr. W. C. Fernelius (6).

The application of this system to homoatomic aggregates is a current problem. The major area of importance to date is that of the closed polyhedral aggregates found in the hypopolyboron ions for which a different numbering system has been used (7). In this case the polyhedron is again viewed down the major symmetry axis, and each plane is numbered clockwise, but the numbering is started

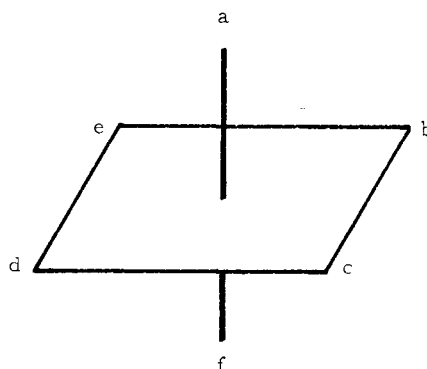


Figure 1. Designations of position in octahedral coordination

for each plane at top center or in the upper right quadrant. This follows the pattern which has been used for the projection formulas for the open framework boron hydrides (8) and that used for the Ring Index (9). This leads to the two different numbering systems for an icosahedron shown in Figure 3.

The IUPAC Commission also favors *closo* rather than *clovo* to indicate such closed polyhedra because of difficulties with pronunciation of *clovo* in some languages. They have also adopted *nido* from the Greek word for nest to indicate open frameworks.

Further problem areas which exist at present are many. Those which seem of greatest urgency to the writer are the following:

- (a) Chains and rings
- (b) Phosphorus
- (c) Ligand resonance
- (d) Designation of coordination number = ligancy = "bindigkeit"
- (e) Derivatives of hypopolyboron anions.

It becomes apparent in further discussions that many of these are interrelated.

The most abundant types of chains and rings in presently known inorganic systems have skeletons consisting of alternating elements such as those found in the siloxanes. Since that area has provided a precedent, this type of nomenclature (10) is generally favored. However, the application of this nomenclature runs into very difficult problems, as can be seen from the following:

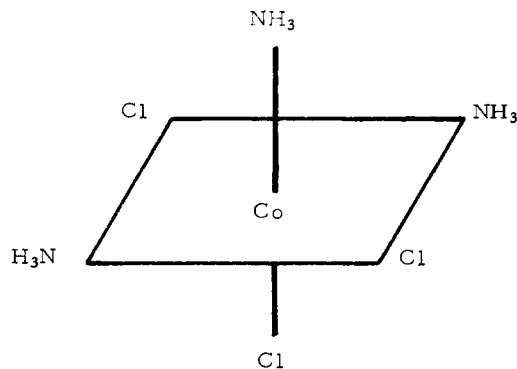
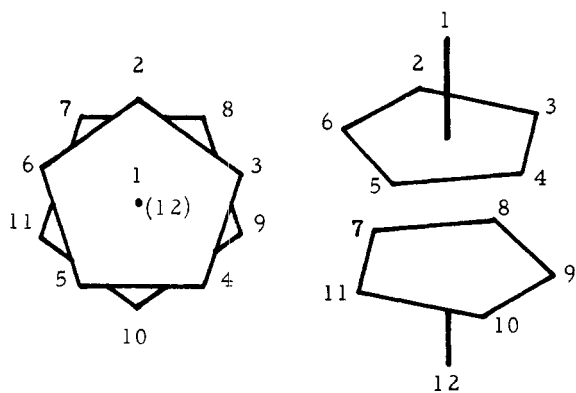
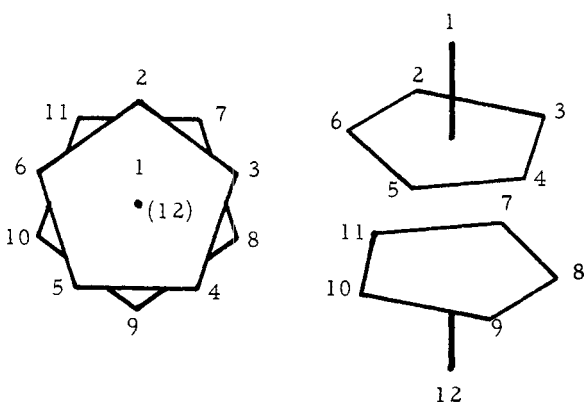


Figure 2. abd-triammine-cfe-trichlorocobalt(III)



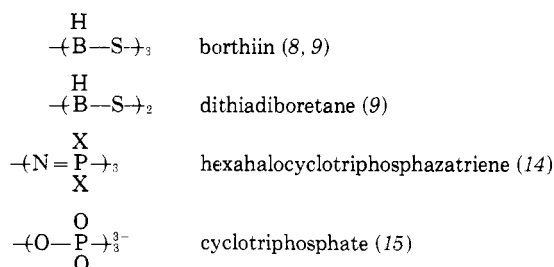
McDonnell and Pasternack (5)



Borane system (7)

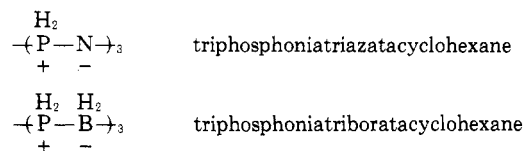
Figure 3. Numbering systems for icosahedra

These precedents would lead to the name cyclotriborazane for $(\text{BHNH})_3$. This has most commonly been called borazine in American nomenclature and borazole in German literature. The name cyclotriborazane has been applied to the substance $(\text{BH}_2\text{NH}_2)_3$ (11). This has also been extended to the similar boron-phosphorus system $(\text{BH}_2\text{PH}_2)_3$ which was called cyclotriborophane (12), which leads to possible confusion with organic cyclophane nomenclature (13). The extent of this problem is emphasized by further examples and the different types of nomenclature which have been used:

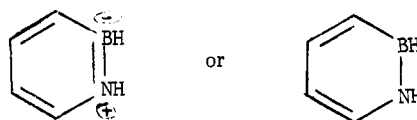


It is noteworthy that although the last two systems are isoelectronic, one has been commonly considered to be double bonded and the other not. This points up the difficulty of depending on bond order for names.

One approach has been to list arbitrary formal charges and to name such structures on this basis.

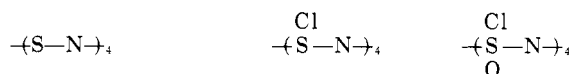


However, in many examples an arbitrary assumption of bonding is necessary to compute formal charge, as in



called borazarene or borazarobenzene (16).

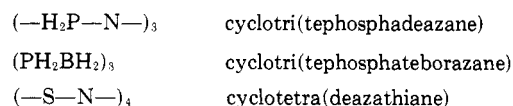
Still greater problems of bond order occur in the following examples, all of which have been written as having S=N double bonds:

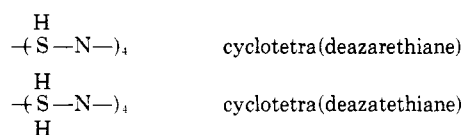


Another system has been suggested by Clifford (17). The suffix "-ane" is used for atoms with no unshared electron pairs, "-ine" for atoms with one unshared electron pair, "-uane" for atoms with two unshared electron pairs, and "-uine" for atoms with three unshared electron pairs. This leads to names which are closer to traditional names. However, with both of these methods, in cases of questionable bond order, arbitrary choices have to be made; in some cases where the bond order is fractional this system appears to be inadequate. It appears to the writer that the most sensible solution to the dilemma involves some sort of designation of ligancy, either directly or indirectly. The IUPAC Commission has tentatively favored the use of Stock numbers to indicate ligancy. However, this leads to confusion with their use for oxidation state. Van Wazer has made a suggestion as follows (15):

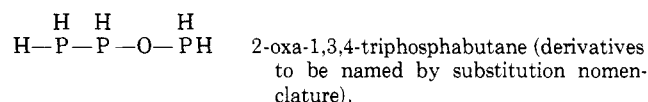
Ligancy or Coordination No.	Suggested Prefix
2	de
3	re
4	te
5	le
6	ne
7	pe

The prefixes might be omitted for the "standard" ligancies for each element assumed in the "oxa-aza" (3) or silicon nomenclature system (10). Some sample treatments of the cases above are:



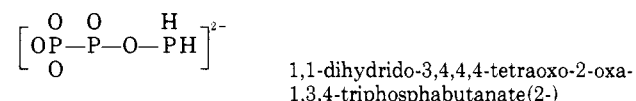
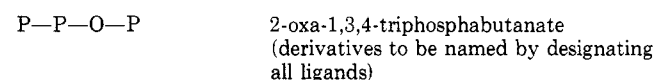


For nonalternating chains, the IUPAC currently favors basing all names on a replacement system based on a hydrocarbon name as is shown by the following example:



Many inorganic chemists would favor the use of the major atom in the skeleton as the basic name instead. For example, the above compound would be called 2-oxatetraphosphane.

For application to ions, the following modification has been proposed by the IUPAC. The suffix "-anate" is assumed to imply an anionic skeleton with no ligands. All ligands then must be designated in the name. This leads to the following applications:



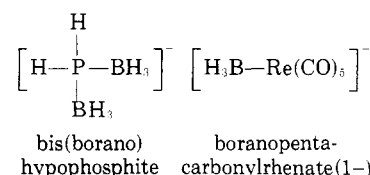
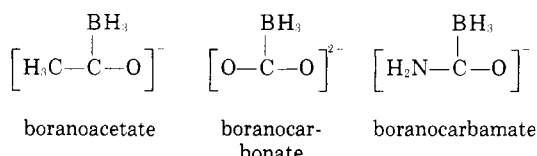
This leads to some conflict with a practice which has been used in Germany and by some British and American chemists for the names of hydropolyboron and hydroaluminum anions in which the "-anate" suffix is assumed to imply saturation with hydrogen. The use of this nomenclature is certainly more euphonious for the simple boron hydride anions but its application has questionable advantage for the more complex cases where the number of hydrogens must be designated and where substitution has occurred as indicated by the following examples:

Formula	Coordination	Type Name	Addition
$\text{B}_{10}\text{H}_{10}^{2-}$	decahydro-decaborate(2-)	decaboranate-10h(2-)	
$\text{B}_{10}\text{H}_9(\text{NH}_3)^{1-}$	amminenonahydro-decaborate(1-)	ammonio-decaboranate-10h(1-)	ammine-decaboranate-9h(1-)
$\text{B}_{10}\text{H}_8(\text{NH}_3)_2$	diammineoctahydro-decaboron	diammonio-decaboranate-10h(0)	diammine-decaborane-8h
$\text{B}_{10}\text{H}_7(\text{NH}_3)_3^{1-}$	triammineheptahydro-decaboron(1+)	triammonio-decaboranate-10h(1+)	triammine-decaboranium-7h(1+)

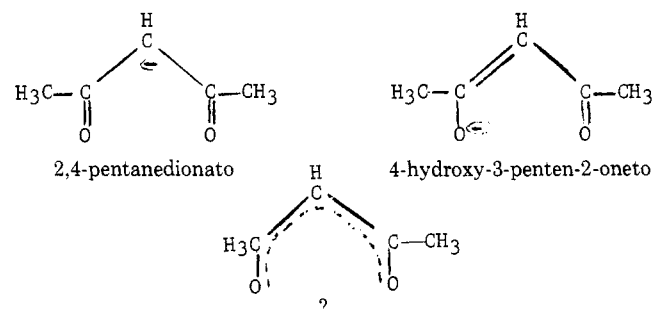
A major difficulty with the boranate names arises in that for cations, if substitution nomenclature is used, the names have an "-ate" suffix which is permissible organic practice but contrary to all current inorganic practice. The only way around this appears to be the use of addition-type nomenclature such as is used in the third column above. However, these difficulties tend to favor straight coordination nomenclature. Another difference in current American practice and the IUPAC recommendations for boron hy-

drides is that the number of hydrogens is given by an Arabic numeral in parentheses in American literature and by a hyphenated numeral followed by a lower case "h" in IUPAC nomenclature. The advantage of the latter is less possible confusion with references. For boronate nomenclature for ions, there is less possible confusion with charge number as shown by the above examples. The IUPAC proposal uses hydrido for all coordinated hydrogen. American practice generally favors hydro, especially when bonded to nonmetals.

Another practice which has been used by several Americans is the use of "borano" to indicate replacement of oxygen by a BH_3 group (18). There is also need for a name for this group as a ligand. Applications of this system are shown in the following examples:



Another problem area involves the designation of ligand resonance as indicated by the following examples (6):



Some have felt that the second name is a more accurate description of the ligand than the first. (However, resonance makes the picture considerably more complex.) Hence, one must assume some knowledge of the chemistry in applying either type of name. A more complex example of resonance and nomenclature problems is shown in Figure 4 which has been named as indicated (19). The proper name by application of current principles would appear to be π -cyclopentadienyl- π -(7,8,9,10,11)[undecahydro-7,8-

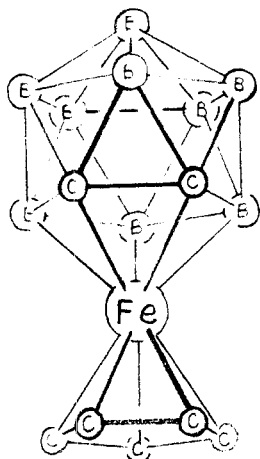


Figure 4. " π -cyclopentadienyl-[1],2,3-dicarbolyliron"
1- π -cyclopentadienyl-1,2,3-ferradicarbadodecaborane(12)

dicarbaundecaborato]iron(III). However, if one includes the iron in the icosahedron, the name would become 1- π -cyclopentadienyl-1,2,3 ferradicarbadodecaborane(12).

One further problem which received partial solution in the IUPAC Commission meeting is the designation of the chirality of chelates. Confusion had arisen because some authors had used the threefold symmetry axis of an octahedron and others the twofold symmetry axis for this designation. The two viewpoints lead to inverted chiralities. Also, different letters have been used to designate this chirality—i.e., R, P, or Δ for a right-hand screw axis and S, M, or λ for a left-hand screw axis. It was agreed at the IUPAC meeting that the twofold symmetry axis would be taken as standard in this case, since it is the only one available for complexes with only four positions chelated. It was agreed that Δ would be used for a right-hand chirality and λ for left-hand. In the cases which have been studied these lead to the R and S of the Cahn-Ingold-Prelog system (20). This is to be checked further and, if found to be uniformly so, R and S are to replace the delta and lambda.

The designation of the chirality of the ligand itself is also a problem. It was agreed that lower case "p" and "m" for "+" and "-" should be used for this rather

than other symbols which have been used to date. This type of problem is likely to become more severe.

The writer would appreciate comments and criticisms in any of these areas in order to obtain the best possible American practice and also for forwarding to the IUPAC.

LITERATURE CITED

- (1) Jorissen, W. D., *et al.*, *J. Am. Chem. Soc.* **63**, 889 (1941).
- (2) Bassett H., *et al.*, *ibid.* **82**, 5523 (1960).
- (3) "The Naming and Indexing of Compounds from Chemical Abstracts," *Chem. Abstr.* **56**, 1N(1962).
- (4) Ewens, R. V. G., and Bassett, H., *Chem. and Ind.* **1949**, 131.
- (5) McDonnell, P. M., and Pasternack, R. F., *J. Chem. Doc.* **5**, 56 (1965).
- (6) Fernelius, W. C., *ibid.* **5**, 200 (1965).
- (7) Adams, R. M., *Inorg. Chem.* **2**, 1087 (1963).
- (8) Schaeffer, G. W., and Wartik, T., "The Nomenclature of Boron Compounds," 125th Meeting, ACS, Kansas City, March 1953.
- (9) Patterson, A. M., Capell, L. T., and Walker, D. F., "The Ring Index," American Chemical Society, Washington, D. C. (1960).
- (10) Drake, L. R., *et al.*, *Chem. Eng. News* **30**, 4517 (1952).
- (11) Shore, S. G., and Hickam, C. W., *Inorg. Chem.* **2**, 638 (1963).
- (12) Goodrow, M. H., Wagner, R. I., and Stewart, R. D., *ibid.* **3**, 1212 (1964); Kokoropoulos, P. K., and Eveslage, S. L., *J. Chem. Doc.* **5**, 91 (1965).
- (13) Wilson, D. J., Boekelheide, V., and Griffin, R. W., *J. Am. Chem. Soc.* **82**, 6302 (1960).
- (14) Shaw, R. A., Fitzsimmons, B. W., and Smith, B. C., *Chem. Revs.* **62**, 247 (1962).
- (15) Van Wazer, J. R., "Phosphorus and Its Compounds," Interscience Publishers, Inc., New York, N. Y. (1958); *J. Chem. Doc.* **4**, 84 (1964); also private communication.
- (16) Maithlis, P. M., *Chem. Revs.* **62**, 223 (1962); Dewar, M. J. S., Kubba, V. P., and Pettit, R. J., *J. Chem. Soc.* **1958**, 3073.
- (17) Clifford, A. F., *J. Chem. Doc.* **4**, 91 (1964).
- (18) Carter, J. C., and Parry, R. W., *J. Am. Chem. Soc.* **87**, 2354 (1965).
- (19) Hawthorne, M. F., and Pilling, R., *ibid.* **87**, 3987 (1965).
- (20) Ingold, C. K., Cahn, R. S., and Prelog, V., *Angew. Chem. (Int. Ed.)* **5**, 385 (1966).