

incorporate CA abstracts in their literature reports or in-house abstract bulletins can therefore count this right as a partially offsetting economic benefit.

The formula for the subscription price is not a simple one. A "scientist served" is not one who by training might be expected to use the CA microfilm, but instead is one who actually does, or who benefits from it directly. Since the microfilm will normally be housed only in one place, it would not be difficult to establish a statistically valid sampling schedule to count the direct users. On the other hand, CA also requires the inclusion of an estimate of the "scientists served" by copies of bibliographies or abstract bulletins that include CA-derived abstracts.

As we have shown, the economics of acquiring and using the CA microfilm are favorable for well-used libraries already possessing complete sets of bound volumes. This new medium should also be attractive to new or branch libraries which can actively use CA but have been hesitant because of the initial costs of the bound volumes, shelving, and floor space; note, however, that the decennial (and later annual) indexes will still have to be purchased and shelved. On our part, we are seriously considering a second set of the CA microfilm for a branch library which has limited floor space but already has the CA indexes since 1947.

The day will come, of course, when the CA-microfilm system that we have discussed here will seem an antiquated method of looking up abstracts. For the immediate future, however, we believe that this system is both useful and economical. We hope that other publishers of sec-

ondary journals will reproduce their reference sets in this manner.

ACKNOWLEDGMENTS

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Nomenclature of Coordination Compounds. Present Status*

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The field of chemical knowledge suggested by the heading "Coordination Compounds" is extensive. Research is currently very active in this field. Consequently, it is important that the underlying principles of nomenclature used in this field be sufficiently broad to handle adequately new compounds resulting from such research. Recently the author attempted to summarize existing practices and needs in the nomenclature of coordination compounds (13). Inadvertently, certain items were overlooked or treated in too little detail. For the sake of completeness, the discussion is contained here.

Designation of Geometrical Isomerism in the Coordination Sphere. Chernyaev (9) used the patterns shown in Figure 1

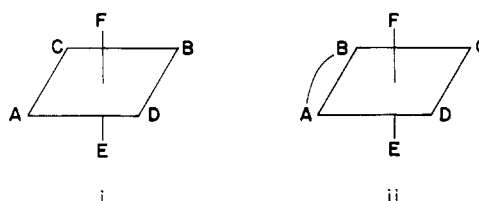


Figure 1.

* Contribution No. RP-65-9 from the Research Dept., Koppers Co., Inc.

for writing formulas and for naming compounds having an octahedral configuration with six unidentate ligands (i) and with one bidentate ligand and four unidentate ligands (ii). By writing formulas and giving names always in the order [ABCDEFPt], he was able to indicate space orientation. For planar configurations the same system was used except that there were no ligands E and F. For the treatment of the coordination compounds of platinum with neutral ligands, where there are many instances of isomerism, "Gmelins Handbuch" (15a) used $\langle \rangle$ to enclose ligands in *trans* positions and $\{ \}$ to enclose those in an equatorial plane (Figure 2).

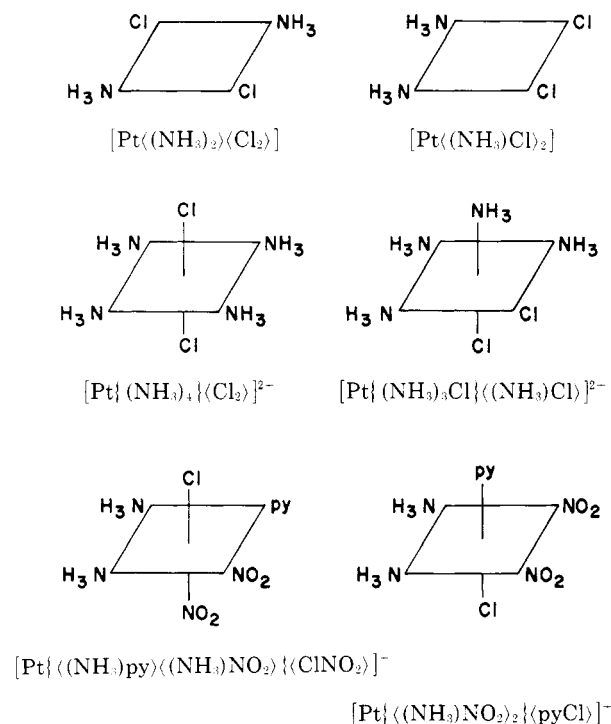


Figure 2.

Numbering Systems for Designating Structures. A numbering system for distinguishing among isomers was introduced by Werner (36) and has been followed by most (but not all) of the authors compiling data about coordination compounds. The conventional system of representation is shown in Figure 3 (3-5, 10, 12, 13, 17, 18, 28, 34, 36-38). Thus, the isomers shown in Figure 4 are designated 1,2 and 1,6 instead of *cis* and *trans*. Similarly, those in Figure 5 are designated 1,2,3 and 1,2,6 instead of *cis* or *fac* (facial) and *trans* or *mer* [meridional (33); peripheral has also been used (7, 17)]. It seems strange that, although the use of numbering systems in organic nomenclature has been widespread, there has been little such numbering in naming coordination compounds. The potentialities of the numbering system seem not to have been realized. This system has been consistently employed (17, 20, 28, 30, 37) only in the use of 1,2 and 1,6 in place of *cis* and *trans*, although Werner (36) used 1,2,3 and 1,2,4 to distinguish between the isomers of the class shown in Figure 5. (The use of 1,2,6 is preferable to 1,2,4 even though the latter

gives the lower series of numbers. The passage from position 1 to 2 to 6 is a continuous path, whereas that from 1 to 2 to 4 is a discontinuous path. Thus, if the three positions were occupied by a linear terdentate group, one does not have the choice between 1,2,6 and 1,2,4 but between 1,2,6 and 4,1,2 or 2,1,4.) Many authors of major compilations have failed even to mention a numbering system (8, 11, 14, 22, 23, 27).

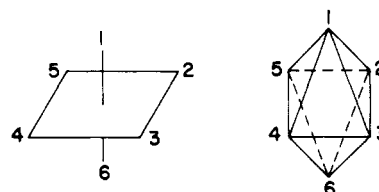


Figure 3.

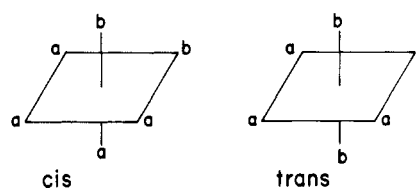


Figure 4.

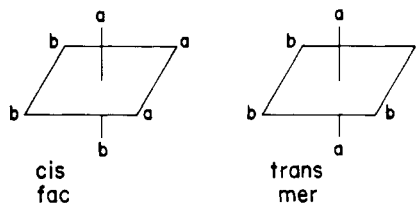


Figure 5.

A few comments about the order of numbers in designating the coordination sites around a central atom are in order. In the conventional system of representation, one begins and ends with a polar position and proceeds around the equatorial positions in a clockwise direction. It is interesting to note that this order transforms readily into another and often useful representation of the octahedral positions (trigonal antiprisms), as shown in Figure 6. This arrangement of numbered positions is identical with that proposed for numbering cage borane compounds (1). No one has stated why this particular arrangement of numbered positions should be preferred to any other. In the first use of a numbering system, Werner (35) designated the axial positions 1 and 2 and proceeded around the equatorial positions in a counterclockwise direction.

Among square-planar compounds, isomers are possible only for those classes represented by the symbolism Ma_2b_2 ,

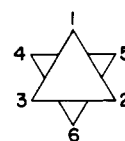


Figure 6.

Ma_2bc , Mabcd (Figure 7), M(AB)cd , M(AB)_2 , and M(AB)(CD) (lower case letters represent monodentate groups and capital letters chelate groups). Since in all cases except Mabcd only two isomers are possible, the terms *cis* and *trans* serve adequately to distinguish between the two. When a numbering system has been used, it is that shown in Figure 8.

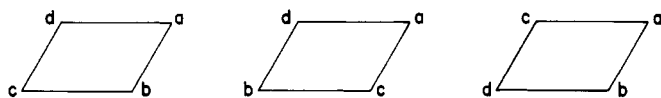


Figure 7.

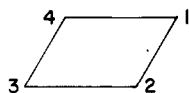
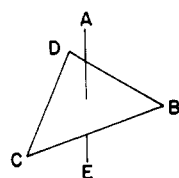
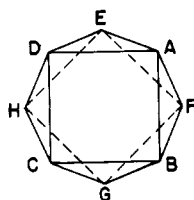


Figure 8.

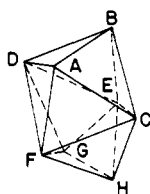
In establishing numbering systems (assigning locant designators) for configurations other than the octahedral and square planar, one hopes for a general procedure of which the accepted patterns are only specific examples. Such a general procedure has been devised by McDonnell and Pasternak (24, 26) and is useful not only for purposes of nomenclature but also for the development of a linear-formula notation system for coordination entities. Their procedure for assigning locant designators to equivalent coordination positions involves, first, locating the highest-order axis of rotation symmetry and then moving down the axis until a point is encountered through which a plane passing perpendicular to the axis also passes through one or more positions of ligand attachment. Designators are assigned to each coordinating position in the plane, moving in a clockwise direction if more than two positions are involved. From the first plane, one moves to the next plane and continues numbering positions beginning with that one nearest (excluding the one directly below) to the last one on the previous plane, moving always in a clockwise direction. This operation is continued until all positions of ligand attachment are assigned designators. Examples of the application of this procedure to specific



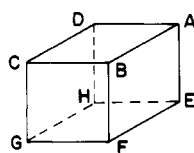
trigonal bipyramid



square antiprism



dodecahedron with triangular faces



cube

Figure 9.

configurations are shown in Figure 9. Note that lower case letters are used rather than numbers as designators, to avoid possible confusion with the many other uses which have been made of numbers for nomenclature purposes.

The only designator systems which have been suggested for bridged compounds (4) apply to the types with two bridging groups and are shown in Figure 10. The appear-

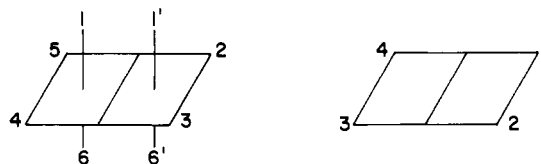
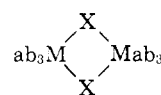


Figure 10.

ance of a paper (21) on the number of theoretically possible isomers of compounds of the type

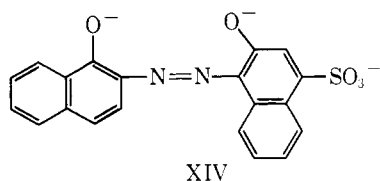
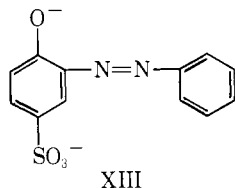
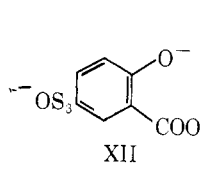
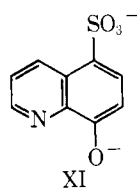
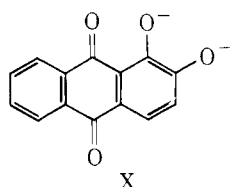
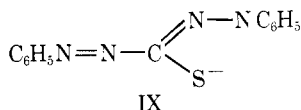
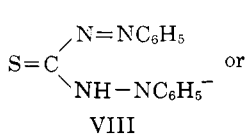
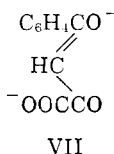
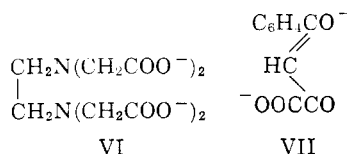
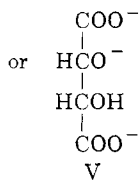
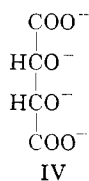
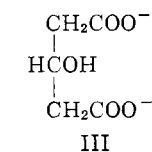
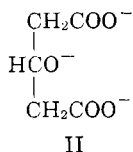
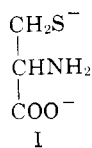


only points up the need for a method to designate the individual isomers.

Designation of a Multidentate Group in Lower Functionality than the Maximum. In the broad area of coordination compounds containing multidentate groups, there are many instances where all of the potential coordination sites on a ligand are not used in coordination. Such ligands include compounds I-XIV as well as polyamines and polypyridines. In some of these, it is obvious that the spatial relationship of the coordination sites is such that all of them could not possibly be attached to the same center of coordination: two nitrogen atoms and the sulfur in VIII-IX, all three of the adjacent oxygen atoms in X, and the SO_3^- and the other coordination sites in XI-XIV. (If the reader is dubious about this statement in any instance, he might try constructing the compound with molecular models.) In others, the participation of all potential coordination sites would either produce considerable strain or greatly limit the variety of ways in which the sites on the coordination center could be involved. However, it is not readily apparent in many cases whether the strength of the bonds involved in coordination can overcome the strain produced in the multidentate coordination. Hence, a nomenclature scheme is needed for designating the particular coordinating sites that are involved when the number is less than the maximum possible.

Actually several accepted nomenclature practices serve to accomplish the desired goal in specific instances.

a. Number of Sites Available on the Center of Coordination. Even though a group like SO_3^{2-} might well be expected to coordinate through two of the oxygen atoms, the stoichiometric composition represented by the formulas $[\text{Co}(\text{NH}_3)_5\text{SO}_4]\text{Br}$ and $[\text{Co}(\text{en})_2\text{SO}_4(\text{OH}_2)]^{2+}$ indicates that only one site remains for the SO_3^{2-} , since each of the NH_3 groups occupies a single site and only six sites are available. In a case where the actual coordinate number was not known as definitely as it is for Co, such a deduction would not be justified.



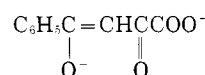
b. *Designation of the Atoms through Which Coordination Takes Place.* One could distinguish among the possible modes of coordination of the cysteine anion (I) thus: cysteinato(2-)*N,S*; cysteinato(2-)*O,S*; cysteinato(2-)*O,N*; cysteinato(2-)*O,N,S* (terdentate). This practice is effective only when the alternate coordination sites do not involve the same kind of atom.

c. *Designation of the Charge of the Coordinated Group.* The ligand $^- \text{OOCCH}(\text{OH})\text{CH}(\text{OH})\text{COO}^-$ is called tarttrato(2-) and $^- \text{OOCCH}(\text{O}^-)\text{CH}(\text{OH})\text{COO}^-$ is called tarttrato(3-). In general, without contrary evidence it might be assumed that the first is coordinated only through the two carboxylato groups, whereas the latter is coordinated through the $-\text{CH}(\text{O}^-)$ and one or two $^- \text{COO}^-$ groups. However, it is conceivable that there would be cases where coordination would be through two charged carboxylato groups and a neutral $-\text{CH}(\text{OH})-$, through only one charged carboxylato and a charged $-\text{CH}(\text{O}^-)-$ group, and through two charged $-\text{CH}(\text{O}^-)$ groups. At present there is no accepted way of indicating these types of coordination. The great weakness of the system of designating the charge on the ion is that the loss of a

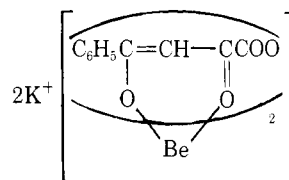
proton at a given position gives no assurance that this position on the ion becomes a site through which coordination takes place.

The above practices suggests some adaptations which might be followed in specific instances. Although ethylenediaminetetraacetic acid normally furnishes a sexadentate ligand with a charge of 4-, there are many coordination entities derived from this acid in which the ligand is quinquedentate with a charge of 3-, such as $\text{Na}[\text{Co}(\text{Hedta})\text{Cl}]\text{H}_2\text{O}$ (6, 25, 29, 32). This salt might be called sodium chloro(ethylenedinitrilo)tetraacetate(3-)cobaltate(III) monohydrate. There remains the need for a name for the ion $[\text{Co}(\text{edta})\text{Cl}]^{2-}$ where the proton on the uncoordinated $-\text{CH}_2\text{COO}^-$ group has been lost. The name chloro(ethylenedinitrilo)tetraacetato-*N,N',O,O',O''*cobaltate(III) clearly defines the situation. In the normal type of ligand (sexadentate with a charge of 4-) the designation (4-) customarily is assumed and omitted in the name.

There remain those situations where the free and the coordinated groups involve the same kind of atom but in a different linkage; e.g.



where the carboxylate group is not coordinated. A previous suggestion (12) was that the position of the coordinated oxygens be designated



potassium bis(benzoylpyruvato- $\text{O}^{\alpha},\text{O}^{\beta}$)beryllate(II)

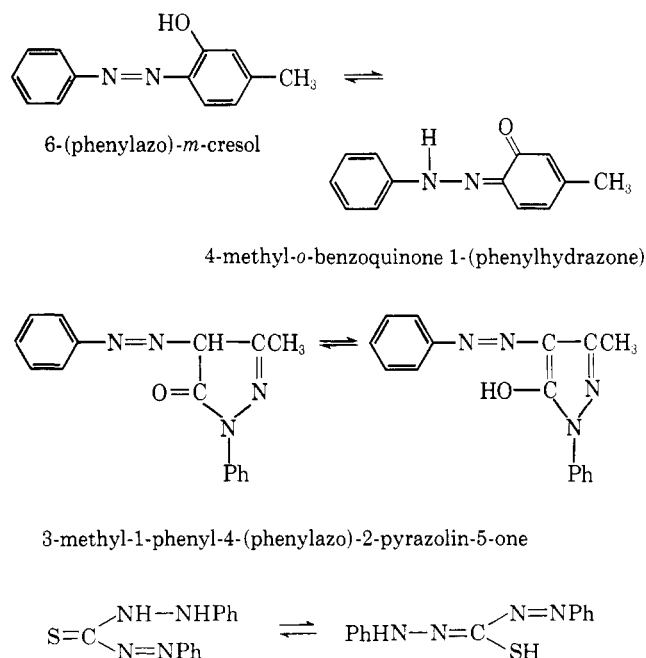
Perhaps the use of numbers to distinguish the oxygens would be better: bis(benzoylpyruvato- O^2,O^4)beryllate, where the numbers signify the carbon atoms in the chain to which the oxygen atoms involved in coordination are attached. Similarly, the various types of coordination of tartrate ions could be indicated: tartrato(3-)- O^1,O^2 for coordination through one COO^- and an O^- on the adjacent carbon atom; tartrato(4-)- O^2,O^3 for coordination through the two O^- s after loss of the protons from the hydroxyl groups; etc.

Finally there is the very vexing problem of a normally chelating group which occasionally coordinates in a lower functionality in a completely different manner: $(\text{CH}_3\text{CO})_2\text{CH}-$ in $[\text{PtMe}_3(\text{dipyridine})\text{HCAc}_2]$ (31) or (1-acetylacetyl)dipyridinetrimethylplatinum (see also ref. 19).

Use of Abbreviations. The most extensive use of abbreviations in giving the formulas of coordination compounds is that in "Gmelins Handbuch." Extensive lists of abbreviations and the corresponding names and formulas are given in two of the volumes (15b, 16). All of the ligand abbreviations used by the editors for individual compounds consist of lower case letters (no capitals) except when it is desired to indicate the undissociated or acid form of an anionic ligand by adding H: dm gH_2 for dimethylglyoxime, dm gH for the usual coordinated ion derived from dimethylglyoxime, and dm g for the doubly

charged ion. Capitalized abbreviations are used in "Gmelins Handbuch" only for the designation of groups of ligands: [Pt Cl₂ Å Ol] for the dichloromonoaminemonoolefinplatinum(II) compounds. Note that the individual ligands are *not* enclosed in brackets but *are* separated from each other.

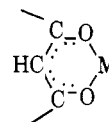
Ligands Which Coordinate in Tautomeric Forms. Several ligands do not coordinate in the tautomeric forms indicated by the customary names. In the instance of 2,4-pentandione (acetylacetone), for example, the anion of the enolic form, CH₃COCH=CH(O⁻)CH₃, is the coordinating species. Hence, the name 4-hydroxy-3-penten-2-onato more accurately represents the coordinated ligand than does 2,4-pentandionate. In the same way, ethyl acetoacetato is less accurate than ethyl 3-hydroxy-2-butenato for the coordinated ligand. Even the hydroxy name is unsatisfactory because the proton of the hydroxy group is lost in the ligand. Similarly, 1,2-naphthoquinone-2-oximato better represents the coordinated ligand than does 2-nitroso-1-naphtholato. Other situations of the same sort are



The last example indicates a ligand which supposedly coordinates in two different ways: a five- or six-membered ring through two nitrogens and a five-membered ring through a sulfur and a nitrogen. The names of the actual coordinated species in any instance would be derived from one or another of the tautomeric forms of the acid form from which the ligand originates.

Care must be exercised in the choice of which tautomeric form to use for a specific ligand. In many instances, such as unsymmetrical β -diketones, it will not be known which of two or more possibilities is the coordinated species. In such cases, it is probably the better practice to use the common form until the question of which form is involved is settled. However, it does seem reasonable to use 4,4'-ethylenediiminobis(2-penten-2-olato) for $[-CH_2N=C(CH_3)CH=CH(O^-)CH_3]_2$ rather than ethylenebis(4-imino-2-pentanonato). Finally, there is no simple nomen-

clature precedent to indicate the electron delocalization represented by



yet this is a very common situation with coordinated ligands. The entire problem requires careful study.

ACKNOWLEDGMENT

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Experimental Designs in Work and Time Studies*

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I. SUMMARY

This expository paper is addressed to the role of statistics in work and time studies involving input to information storage and retrieval systems. General statistical techniques for gathering data by observation and by experimentation are discussed. Examples are given to illustrate the importance of proper sample and experimental design with regard to reliability and cost.

II. GENERAL COMMENTS

One obtains statistical information in time and work studies to measure characteristics associated with individuals and other system components, and to provide a rational basis for selection among alternative system components. Management must specify system properties of interest such as quality, rate of work, and cost. Furthermore, specific attributes of these properties must be chosen prior to observation or experimentation. For example, quality of indexing may be described by indexing accuracy or consistency (1). Analysis should be planned to yield the best information upon which to base decisions. For instance, statements of indexing accuracy are more valuable to management if accompanied by statements concerning the effect of indexing accuracy on missed documents and false drops (2).

System characteristics are generally measured by averages, totals, proportions, and measures of variability. A measure of dispersion should accompany each average, total, or proportion to provide a better description of the population studied. For example, average daily room temperature of 70° F. has little meaning for describing work conditions if the temperature ranges from 50 to 100° F. during the day. Average accuracy for an entire group of indexers may be high, but one or more individuals may differ widely from the average. The standard deviation is the most common measure of dispersion. (Standard deviation for a finite population is $\sigma = [\sum(X - \mu)^2/N]^{1/2}$, where μ is the population mean, X is an observation from the population, and N is the number found in the population.) The standard error of a mean (average) is measured by the standard deviation divided by the square root of sample size. In a sense, standard error is a description of reliability of statistical estimation.

III. SAMPLE DESIGN

Observational information is obtained by examining a portion of a population in order to make generalizations concerning the entire population. The generalizations may be estimates of population characteristics or tentative hypotheses concerning the population under investigation. Generally, no attempt is made to modify or control any aspect of the system being observed. Statistical sampling theory deals largely with seeking a balance between reliability and cost of sample estimates, while sample design is the mechanism for accomplishing this. Sample design includes the sample plan and estimation procedure.

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