[CONTRIBUTION FROM THE CHEMISTRY DEPARTMENT OF ANTIOCH COLLEGE] THE NOMENCLATURE OF PARENT RING SYSTEMS^{1,2}

BY AUSTIN M. PATTERSON Received July 30, 1928 Published November 6, 1928

General Principles

1. Any attempt to construct a strictly logical system of names for the large number of parent ring systems now known seems impractical, at least so far as common use is concerned. Brief special or "trivial" names (Trivialnamen) for many systems have become well established and have proved their convenience, while systematic names tend to become long and to be complicated with numbers and letters in order to distinguish isomers.

J. J. Sudborough, J. Indian Inst. Sci., 7, 145–195 (1924); C. A., 19, 825–826, has developed a scheme of nomenclature for ring systems. He names each form by selecting a peripheral ring as a basis and indicating how it is bridged, which is possibly the simplest method that could be chosen. According to his plan the name for what has been called 9,10-diphenylenephenanthrene (a six-ring parent hydrocarbon) is "5B-1:1:22, 2:2:15, 3:3:8, 9:9:14, 16:16:21,-cyclo-hexacosa- $\Delta^{4:6:10:12:17,19:23:25}$ octene." T.S. Wheeler, Chem. News, 126, 33–35, 49–50, 66–67, 113–115 (1923), proposes to proceed in a linear manner from one component ring to another, characterizing each on the way. His name for the compound just mentioned is "hexar-3,4-hexar'-2,3hexar''-2,3-hexar; 4',5'-hexar; 4'',5''-hexar." It is hard to imagine that such names as these could ever come into extended use. They might conceivably be employed in a telegraphic code or in some systematic form of indexing.

2. On the other hand, it would not be wise to coin a special name for each parent compound known. The number of such names would be large. Ingenuity would be taxed to find names that should aptly characterize each one. Such names make demands on the memory or require access to a reference book, and they throw little or no light on structural relations.

3. Consequently, any practical system of naming parent ring compounds will be a compromise between brevity and logical system. A parent compound that has an important family of derivatives or that has become prominent for any other reason should have a name of convenient length. On the other hand, it is an advantage to name ring systems so as to indicate

¹ In memory of Ira Remsen.

² The substance of this article was communicated in manuscript form in March, 1926, to the other members of the Comité de Travail on Organic Nomenclature of the International Union of Pure and Applied Chemistry. It has now been revised for publication, with comments on an article since published by Prof. Robert Stelzner. The writer found, on visiting Hofmannhaus (Berlin) in 1925, that the workers there and those of *Chemical Abstracts* had arrived independently at some of the same ideas, especially as regards the naming of heterocyclic systems, while differing rather definitely on certain points. He takes this opportunity of expressing his appreciation of the cordial attitude and coöperation of Professor Stelzner, Professor Prager, Doctor Kuh and Doctor Stern. their structure, either as to component atoms (as in "triazole") or as to component rings (as in "benzopyran"). "Triazole" happens to be both brief and systematic. It should be possible to name some compounds in more than one way; for example, it is useful to be able to say that camphane is, 1,7,7-trimethyl-norcamphane and that norcamphane is bicyclo[2.2.1]heptane. If our names are to be both convenient and logical, there must be some flexibility. In what follows, only the possibilities for systematic naming will be discussed.

4. Existing names and usages should be conserved in so far as they can be adopted into a fairly consistent general plan. Nomenclature in use must be reckoned with. No matter what is substituted for it, it will persist for a certain time. The more such confusion can be avoided, the better. Really discredited names will slowly drop out.

5. In general, the presence of all the component rings of a ring system should be clearly indicated in its name. It is very easy to disguise the presence of rings by using a prefix denoting a multivalent radical. Thus, thiodiphenylamine suggests two separate benzene rings but actually is the name of a three-ring complex; benzoyleneguanidine contains a tworing complex; while malonylurea, at first sight an aliphatic compound, is the derivative of a six-membered ring. Such names not only do not express clearly the nature of the ring system; they often prevent a compound from being indexed with other compounds of related structure and they often fail to provide sufficiently for naming derivatives. There are exceptions to the principle stated at the head of the paragraph. Names like malonylurea have their uses and should not be suppressed. Moreover, some compounds, as lactones and acid anhydrides, are more suitably named with reference to the compound from which they are formed than with reference to the cyclic system which they contain. Also, it may at times be desirable to use a multivalent radical prefix to name a bridge, as in 1,4-imino-benzene. Nevertheless, the general principle of naming compounds so as to recognize clearly all rings present, unless there is definite reason to the contrary, seems valid.

6. There should be a clear distinction between the names of ordinary substituting atoms or radicals and the names of atoms or rings used in forming the names of parent ring systems. This becomes immediately evident when one attempts to index substances under the names of their parent compounds. "Thio," for example, is used to denote the replacement of oxygen (or sometimes hydrogen) by sulfur; but it may also denote the replacement of methylene by sulfur in a ring (as in "thiodiazole"). Similarly, "oxy" may mean replacement of hydrogen by oxygen (or even by hydroxyl), and also the replacement of methylene by oxygen in a ring. In order to avoid confusion with the ordinary meanings of oxy-, thio, azo-, etc., it is recommended that the forms oxa-, thia-, aza-, etc., be em-

ployed to indicate the presence of hetero atoms in a ring (the a being dropped before a vowel).⁸

Thus one would have thiadiazole, oxadiazole (which is more euphonious than oxdiazole), thiazine, oxazine. Combining forms to indicate the presence of rings in a complex are usually clear enough (for example, benzo-, naphtho-) and not liable to confusion with the names of corresponding radicals (as phenyl, phenylene, naphthyl).

7. There is a useful analogy between the naming of individual compounds as derivatives of a parent compound and the naming of complex ring systems as derivatives of a less complex parent system. For example, the names dichloro-ethane and dibenzocarbazole are analogous, even though in the one case there is replacement of hydrogen by chlorine, while in the other case two benzene rings are regarded as having been "fused" with the carbazole complex (a highly theoretical assumption). It is worth while to follow out this analogy (see especially p. 3081).

8. With regard to terminations, three general methods of naming parent ring systems are in vogue. The first is illustrated by such names as ethylene oxide, tetramethylene, hexamethylenetetramine. It consists in juxtaposing the names of the radicals or atoms that make up the system without much regard to consequences, and must therefore be regarded as rather unsatisfactory, especially for naming derivatives. The second is based on analogy with aliphatic hydrocarbons. According to it, saturated carbocyclic systems form names ending in -ane, while unsaturation is indicated by -ene, -diene, etc., depending on the number of double bonds present; examples: cyclopropane, bicyclononene, spiroheptadiene. Such names are convenient and systematic and are much used for non-aromatic systems. The third method, which is used for the great majority of ring

⁸ As previously stated, the proposals in this article were made to the Comité de Travail on Organic Nomenclature in 1926. A similar scheme for the use of oxa-, thia-, aza-, etc., was published in the same year by Professor R. J. Stelzner (*Literatur-Register* der organischen Chemie, 5, ix-xv). The *a* endings had previously been used by Bouveault (Ber., 31, 3373 (1898); Beilstein's "Handbuch," 3rd ed., Vol. 4, p. 1 (1899)); Ingold (J. Chem. Soc., 125, 87 (1924)), Sudborough (J. Indian Inst. Sci., 7, 182 (1924)), and probably others.

Both Professor Stelzner and the writer would employ the principle for various classes of heterocyclic ring compounds (see the following pages). It might also be extended to open chains of mixed composition. For example, the compound CH_3N = NNHCH₃ could be called 2,3,4-triaza-2-pentene, semicarbazide would be 1,2,4-triaza-butan-3-one, and $CH_3OCH_2OCH_3$ would be 2,4-dioxapentane. Such a nomenclature would provide much simpler names for certain polyethers, polysulfides, etc., than we have at present; this is mentioned merely to show its possibilities. The same idea has already been used to some extent for aliphatic silicon compounds (for example, silicononane, $C_3H_{20}Si$).

The use of such forms as thiona- $(-SO_{-})$ and sulfona- $(-SO_{2-})$ in making ring names does not seem advisable. It would be better to use thia-(-S-) and treat the sulfoxides and sulfones as oxides of the fundamental form.

systems, assigns to unsaturated hydrocarbons the ending -ene, no matter what the degree of unsaturation, and to heterocyclic compounds such endings as -ine, -ole and -an. This system has arisen largely in connection with aromatic and quasi-aromatic compounds, in which a stage of low saturation is looked on as the fundamental form, as naphthalene, pyrrole, furan. Increasing stages of saturation are usually represented by "hydro" or "hydride" names (as, dihydronaphthalene) but in some cases by special endings (as, pyrroline, pyrrolidine). Although the last two methods are to some extent contradictory,⁴ a continuation of both seems inevitable.

Simple Carbocyclic Rings (Class A I)⁵

The Geneva names for monocyclic saturated hydrocarbons, namely cyclopropane, cyclobutane, etc., and also the corresponding names cyclopropene, cyclobutadiene, etc., have been well accepted. They are unquestionably superior to the older names such as trimethylene, and they also seem to be preferred to Zincke's names (R-pentene, etc.), which are seldom seen nowadays. The "cyclo" names are clear and systematic and they correlate cyclic with aliphatic compounds. Nevertheless, it should be pointed out that these names are unlike those of the majority of ring systems (see p. 3076). There is a chemical reason for this in the distinction between aromatic and non-aromatic properties. It would, however, conduce to uniformity of cyclic names and numberings if we had, for example, a basal name for cyclopentadiene and named cyclopentene and cyclopentane as the dihydro and tetrahydro compound, respectively. The "cyclo" names do not yield very convenient prefixes for use in naming complex systems. For instance, derivatives of the compound



exist, and it has been called "cycloheptano-I

pyrazole" by its discoverer. Less saturated stages would presumably be called "cycloheptenopyrazole," "cycloheptadienopyrazole," etc. Thus there is a multiplication of prefixes and parent forms, which does not occur with benzo-, naphtho, pyrrolo-, etc. In the *Chemical Abstracts* indexes the form of lowest saturation, that is, cycloheptatrienopyrazole, has been called "cycloheptapyrazole" and the more saturated forms are treated as hydro derivatives, but the name is not altogether satisfactory, as it might be taken to imply the combination of seven pyrazole rings into one grand cycle. There is therefore a certain lack due to the

⁴ For a discussion of one difficulty caused by their conflict, see Patterson, THIS JOURNAL, 47, 553-554 (1925).

⁵ The classification is that adopted in "Proposed International Rules for Numbering Organic Ring Systems," THIS JOURNAL, **47**, 543-561 (1925). absence of brief names for cyclopropene, cyclobutadiene, cyclopentadiene, cycloheptatriene, etc.

Simple Heterocyclic Rings (Class A II)

About a dozen three-membered heterocyclic rings are known. Those that are named at all are given such titles as ethylene oxide, hydrazimethylene (see general principle 8, p. 3076); there is no systematic way of naming them. Almost the same is true of the four-membered rings, of which there are about two dozen. Some are called trimethylene oxide, trimethylene sulfide, etc.; others are called betaine, thetin and "phosphorbetain." Hale⁶ has coined the name "urete" for a four-membered parent ring, $C_2H_2N_2$, and the *Chemical Abstracts* indexes, following this lead, have adopted *-ete* as an ending for other four-membered rings (azete, triazete).

For five-membered rings proposals made by Widman,⁷ Bouveault⁸ and others have found their way into use. The ending -ol or -ole appears in such names as pyrrole, imidazole and even dioxole (which is non-nitrogenous). It conflicts with the ending -ol for alcohols and phenols (hence the modified spelling -ole), but its use to denote a five-membered ring is well known. Perhaps the most easily understood names are those that prefix to this ending syllables denoting the kind and number of hetero atoms present, thus: diazole, triazole, thiodiazole (better, thiadiazole). The suffixes -oline and -olidine are in use for the hydrides of these rings (as pyrroline, pyrrolidine).

In the field of six-membered rings are found names corresponding to the above systematic names for five-membered rings, but with the suffix *-ine* or *-in* replacing -ole (or -ol), as: triazine, oxazine, thiodiazine, dioxin (the latter being non-nitrogenous). Thus the ending -ine (or -in), although regarded as properly the ending for bases, has a specific sense in which it indicates a six-membered ring. For rings of more than six members there is no system in use, beyond names like trimethylene tetrasulfide, diethylene tetrasulfide, trimethylene-ethylenediamine, etc. (see general principal 8, p. 3076). Crowther, McCombie and Reade⁹ have used the name "dioxazseptane" for a seven-membered ring.

Such is the present state of affairs. Convenient special names like pyrrole, thiophene and pyridine are not likely to be displaced, but systematic names are needed for many simple heterocyclic systems. In what way can progress be made? Ingold¹⁰ has proposed to form names according to the first method mentioned under general principle 8 (p. 3076), as trimethyleneimine, oxatrimethylene (trimethylene oxide), 1,3-dioxadi-

- ⁷ Widman, J. prakt. Chem., [2] 38, 189 (1888).
- ⁸ See Beilstein's "Handbuch," 3d ed., Vol. 4, p. 1.
- ⁹ Crowther, McCombie and Reade, J. Chem. Soc., 105, 933-947 (1914).
- ¹⁰ Ingold, *ibid.*, **125**, 87-88 (1924).

⁶ Hale, This Journal, 41, 376 (1919).

3079

imine. He deals with four-membered rings only, but the same principle could of course be extended. The objections to the plan are that the names are made up of names of radicals and atoms and therefore do not present the parent ring systems clearly as entities (see general principle 5, p. 3075), that hydrogenation or dehydrogenation changes the names rather profoundly, and that the names do not lend themselves well to indexing or to the formation of prefixes for naming more complicated forms. Stelzner¹¹ would use the combining forms oxa-, thia-, etc., referred to under general principle 6 (p. 3075), prefixing them to the name of the carbocyclic form of the same number of members and same saturation. Thus, ethylene oxide would be oxacyclopropane; pyrrole would be aza-5-cyclopentadiene-1,3. This plan has much to recommend it, being easy to understand and apply. It should at least prove useful in systematic works of reference. The disadvantages of the method are: (a) the names of bases are not given a characteristic ending, but terminate like those of the hydrocarbons. This might perhaps be obviated by arbitrarily adding the ending -ine. Thus, ethylenimine might be called, not azacyclopropane but azacyclopropanine. (b) Tautomeric compounds such as pyrrole, isopyrrole and pyrrolenine (which Stelzner calls, respectively, aza-5-, aza-1- and aza-2cyclopentadiene-1,3) do not have the same number for the hetero atom. This could be remedied easily by assigning varying positions to the double bonds, and in the writer's opinion this would be preferable, as chemists are accustomed to regard the position of the hetero atom as fixed. Stelzner, however, does not favor this solution and it could not well be applied to complex systems like indole and pseudo-indole (belonging to Class B; see p. 3084). (c) The names tend to be rather long and do not yield convenient combining forms if these should be desired for naming complex systems.

An alternative method would be to improve and extend the existing practice of using characteristic syllables to indicate the number of members in the ring. In spite of objections that might be urged against it, this method furnishes many neat names and combining forms (as triazole, triazolo-, oxazine, oxazino-). With a precedent already set for et (four members, compare "tetra") and with ol (five members) and in (six members) already confirmed by usage, it would only be necessary to supply three syllables more to cover all but rare cases. These might be ir (from "tri," reversed) for three members, ep (from "hepta") for seven members, and oc (from "octa") for eight members. The series could be extended if desired by selecting on (from "nonus") for nine members, and ec (from "deca") for ten members. Some of these syllables are not acceptable as endings because of prior use (for example -ol for alcohols) but they may be used in the middle of a name without objection. Examples of the resulting names and combining forms are: oxirene, oxirane (ethylene oxide),

¹¹ Stelzner, "Literatur-Register der organischen Chemie," 5, ix-xv (1926).

oxiro-, azetine, azeto-, oxetane (trimethylene oxide), oxeto-, tetrazepine, tetrazepo-, 1,2,4,6-tetrathiepane (trimethylene tetrasulfide), s-tetrazocanine (tetramethylene tetramine), 1,3,5-triazocanine (parent substance of acetonylbiuret). In the last two cases the ending -ine (characteristic of names of bases) has been attached to names that would otherwise have terminated in -ane. The wide use that such names have attained in the five- and six-membered series illustrates the fact that an extremely compact systematic name is often better than either a more extended systematic name or an arbitrarily coined special name.

Order of Hetero Elements.—In the "Rules for Numbering,"¹² the order of hetero elements is determined according to a descending order of groups in the periodic table and an ascending order of atomic numbers in each group. This results in the following order for commonly occurring hetero elements: O, S, Se, Te, N, P, As, Sb, Si, Sn, Pb, Hg. A majority of names in the literature conform to this order (cf. oxazine, thiodiazine), but not all (cf. thioxole). In the judgment of the writer it is better than an order based on valence, since the latter is a variable property. It is important that changes in valence, hydrogenation, etc., should not affect names and numberings profoundly.

Distinguishing Isomers.—Various methods are now employed to distinguish isomeric heterocyclic rings, among which may be mentioned: Arabic numerals (e. g., 1,2,4-oxdiazole), Roman letters (e. g., pyrro[ab]-diazole), Greek letters (e. g., γ -pyran), abbreviations denoting structure (e. g., as-triazine), prefixes (e. g., isothiazole), suffixes (e. g., pyrrolenine), and different special names (e. g., pyrazole and imidazole). In important cases the isomers should probably have different names; in the others Arabic numerals indicating the positions of the hetero atoms seem to be clearest, though sometimes a little cumbrous. The numerals are often made to indicate at the same time the position of methylene groups when this is necessary. It would be well, however, to reserve some prefix, preferably *iso*-, to indicate isomerism caused by change in position of hydrogen. For example, if the two isomers of pyrrole had not already established names they might be called, respectively, 2- and 3-*iso*pyrrole



Complex Ortho-Fused Ring Systems (Class B)

Many systems of this class have well recognized special names, as naphthalene, phenanthrene, quinoline. Where such names do not exist it is

¹² Patterson, This Journal, 47, 545 (1925).

customary to build up names from the simpler systems which may be regarded as present in the complex system to be named, as benzo-pyran. As the Meyer-Jacobson "Lehrbuch"¹³ points out, there is no generally observed system for doing this. Certain principles may, however, be laid down (some of these are corollaries of general principle 7, p. 3076):

(1) Other things being equal, the largest component having a simple name is to be taken as the parent form, to which the other rings or complexes are regarded as being attached. Thus we would naturally say "pyridocarbazole," not "carbazolopyridine."

(2) A heterocyclic component is to be preferred to a carbocyclic as the parent form, even though smaller. Thus we say "naphtho-thiophene," not "thiophenonaphthalene."

(3) A nitrogenous component, if present, is preferred as the parent form, in order that the name of the system may have a termination indicating a base. Thus it is customary to say "furo-pyrrole" not "pyrrolofuran."

(4) No ring in the complex system should be expressed more than once in the name of the complex.¹⁴

Thus, "naphthacridine" most appropriately designates a five-ring system composed of a naphthalene complex and an acridine complex, united by ortho fusion. The name has been used (unwisely, as it seems to the writer) to designate a four-ring system in which a naphthalene complex and an acridine complex exist, to be sure, but having one benzene ring in common; in other words, there is overlapping and this benzene ring is expressed twice in the name. Meyer and Jacobson^{14b} also disapprove of the overlapping method ("the Gräbe-Skraup use of prefixes") and favor the non-overlapping plan (of Hantzsch and Widman).

(5) Like components should be treated alike if possible. Thus, for the system



the name "dibenzanthracene" would be chosen in preference to "naphthophenanthrene" (this is analogous to the choice of "diphenylmethane" in preference to "benzylbenzene)."

(6) Other things being equal, the parent form should be so chosen as to make the "substituents" as simple as possible. Like (5), it would lead to the name "dibenzanthracene" in preference to "naphthophenan-

¹⁸ Meyer and Jacobson, "Lehrbuch der organischen Chemie," 1920, Vol. 2, Part 3, p. 31.

¹⁴ (a) Cf. Patterson, THIS JOURNAL, **39**, 1632 (1917); (b) Meyer and Jacobson, **1920**, Vol. 2, Part 3, pp. 31-32, 1105.

threne." This principle is questionable, since it might lead to longer names, for brevity is of great importance in naming ring systems.

(7) For each important "substituent" component there should be a recognized prefix. In general this would be formed from its name with use of o as final vowel; as, pyrrolo-, pyridino-, fluoreno-. Some well established contractions should be accepted, as anthra-, benzo-, naphtho-, but none that is ambiguous; thus, it would be better not to use pyrazo- at all but to employ the more exact pyrazolo- and pyrazino-. It should be noted that the prefix pheno- or phen- has been used to indicate *two* benzene rings (as in *phenazine*, *phenoxazine*) and also in other ways (as in *phenanthrene*, *phenobarbital*); the natural conclusion is that "benzo" should always be used when one wishes to denote the attachment of a single benzene ring by ring fusion.

(8) In accordance with the aromatic nature of the compounds, the basal names of ring systems of this class are usually given to the *least* saturated form, stages of greater saturation being named as hydro derivatives or hydrides. In the writer's opinion it is well to adhere to this rule even when a non-aromatic ring is a component of such a system. For instance, it seems simpler to have one combining form "cyclopenta-" or "cyclopento-" for the five-membered carbon ring than to attempt to distinguish between cyclopentano-, cyclopenteno- and cyclopentadieno- when this ring is attached, say, to a quinoxaline complex (*cf.* "cycloheptano-pyrazole", p. 3077). The whole system can be reduced to lowest hydrogenation and hydro derivatives indicated.

(9) The true names of components should be used in forming the name of the complex system. This statement seems obvious yet it is frequently disregarded in practice. For example, the system



has been called *peri*-naphthindene, yet it does not contain the indene structure as a component; it is *peri*-benzonaphthalene.¹⁵

Again, the form



¹⁵ Meyer and Jacobson and Stelzner and Kuh have sought to avoid naming "peri" systems in the same manner as ordinary ortho-fused systems because the two classes are not isomeric; *e. g., peri*-benzonaphthalene is $C_{13}H_{10}$, while the ordinary benzonaphthalenes (anthracene and phenanthrene) are $C_{14}H_{10}$, but the writer feels that any advantage gained by distinguishing the two classes by such prefixes as benzo- and benzi-, or benzo- and benzolo-, are at least offset by corresponding drawbacks.

Nov., 1928 The nomenclature of parent ring systems

is not a benzotriazine, even though it is an isomer of those systems; it is a pyridopyridazine.

Distinguishing Isomers.—As in the case of simple heterocyclic rings, isomers in the complex ortho-fused systems are at present distinguished in a very opportunist way: by numbers, by Roman, italic or Greek letters, by prefixes (as iso-, pseudo-, lin-, ang-), by different special names, etc. Here again the more important isomers may well have names of their own (as anthracene and phenanthrene). For the other cases there should be some general system. Following out the analogy of general principle 7 (p. 3076), it would seem that such a system should be based on the numbering of the "parent" component¹⁶ and that of the "substituent" components. The "Rules for Numbering"¹⁷ would furnish a standard for this purpose. The following plan is suggested: for the numbering of the "substituents" retain their Arabic numerals; for the numbering of the "parent" component start with the side 1,2 and letter the sides of the complex with Greek, or rather (since chemists seem to be less and less familiar with that language), small italic or Roman letters. Letter every side, even where there are no numbered positions, as fusion may occur on any side. Then use only such of these symbols as are needed to indicate where the fusion has occurred. Place them in the heart of the name, as Baeyer did in naming the "bicyclo" compounds, so as to avoid confusion with other symbols. A few examples will make the plan clear:



As all six positions on the benzene ring are equivalent, it is not necessary to introduce numbers in the benzoquinoline names. In the last three examples the order of the numbers (1,2 and 2,1, etc.) indicates whether

¹⁶ Cf. Bally and Scholl, Ber., 44, 1662-1665 (1911).

¹⁷ Patterson, This Journal, 47, 543-561 (1925).

308**3**

the numbering of the "substituent" (naphthalene) travels with or against that of the "parent" on the side where fusion occurs.¹⁸

This method of distinguishing isomers has been experimented with in the indexes to *Chemical Abstracts* and has been found satisfactory and of very general application. It applies to "peri" systems, in which case more than one letter is used (see the last example on p. 3083), and to the rare spiro systems of this class.

Use of the Aza-, Thia-, etc., Names.—For heterocyclic systems of this class, Stelzner proposes to use the same method as already described (p. 3079), that is, basing the name on the corresponding carbocyclic form and using prefixes to indicate the hetero atoms. The plan has the same advantages and disadvantages as outlined above (p. 3079), with two additional considerations. The first is, that it does not remove the necessity for coining names for the carbocyclic compounds, which must still be handled by some other method. The second and more serious consideration relates to the effect of the plan on complex ring systems differing only as to the position of hydrogen atoms. The remedy suggested on page 3079 cannot be applied here. Indole, for example, would be (if the "Rules for Numbering" are followed) aza-1-indene, while ordinary pseudo-indole (indolenine) would be aza-3-indene.



This causes the numberings of the two systems to become quite different, although they are desmotropes. Chemists would naturally much prefer that the nitrogen atom retain the number 1 in both cases.

Simple Bridged Systems (Class C I)

Carbocyclic Systems.—The method proposed by Baeyer¹⁹ for naming and numbering the carbocyclic systems of this class has been adopted into general use. One very slight change could be made to advantage, namely, reversing the order of the figures in the middle of the name: *e. g.*, bicyclo[0,1,3]hexane would become bicyclo[3,1,0]hexane. As Baeyer himself remarked, the order of these figures is not significant; but the *decreasing* order is in accord with Baeyer's numbering of the system and also is the appropriate one in Class C III (see p. 3086).

¹⁸ The orientations here given are intended to show relationship to quinoline. Each ring system has, according to the "Rules for Numbering," an orientation and numbering of its own and the symbols in the heart of the name (in brackets) have nothing to do with this.

¹⁹ Baeyer, Ber., 33, 3771-3775 (1900).

Nov., 1928 THE NOMENCLATURE OF PARENT RING SYSTEMS

Heterocyclic Systems.—The "Rules for Numbering" extend the Baeyer method to heterocyclic systems, choosing as low numbers as possible for the hetero atoms. Such systems are named conveniently by using the prefixes "aza-," "oxa-," etc., in connection with the Baeyer names for the corresponding carbocyclic forms, as the difficulty about tautomers referred to under Class B (see p. 3084) does not arise. Thus, nortropidine



may be called aza-8-bicyclo[3,2,1]octene-3; or, if it seems desirable to have all such compounds appear together under "Bicyclo-" in an index, it may be called bicyclo[3,2,1]-az-8-octene-3. If the characteristic ending for the names of bases be added, the termination would be changed from "-octene-3" to "-octen-3-ine."

Complex Bridged Systems

Systems Related to Class B.—The "Rules for Numbering" have distinguished as "Class C II" a small class of parent compounds which may be regarded as formed by throwing a bridge or bridges across an ordinary ortho-fused system of Class B (naphthalene, anthracene, quinoline, etc.). These systems, when not too complex, may be suitably named by prefixing the name of the bridge to the name of the corresponding Class B form. Thus, the system



would be named ethyleno[1,4]isoquinoline. It is questionable whether the more complicated members of this class will ever need to be named as parent compounds.²⁰

It should be remarked that the plan just proposed does not give to bases names ending in -ine if the nitrogen is in the bridge. For example the system



would be imino[1,4]naphthalene. On this account it might be better in such cases to indicate the bridge last and choose the name naphthalen-[1,4]imine.

²⁰ See some of the formulas given under Class C II in THIS JOURNAL, 47, 559 (1925).

3085

Tricyclo and Tetracyclo Systems (Class C III)

These systems are numbered, in the "Rules for Numbering," by a simple extension of the Baeyer method. If these rules are adhered to, names similar to the Baeyer names for bicyclic systems can be given to them, with these differences: (1) the name must now begin "tricyclo" (or, rarely, "tetracyclo," etc.) and (2) the additional bridge or bridges must be designated as to number of members and position. This can most simply be done by inserting additional numbers in the middle of the name, with indices to show where the bridge ends are attached.²¹ For example, the system



may be called tricyclo $[4,1,1,0^{2,4}]$ octane, the zero denoting that the additional bridge contains no atoms and the "2,4" showing where it is attached. It will now be seen why the *decreasing* order of announcing these numbers was preferred on a previous page (3084).

Heterocyclic systems of this class would be named in exactly the same manner as the simple heterocyclic bridged systems (see p. 3085).

Simple Spiro Systems (Class D I)

Simple spiro systems containing one or more spiro atoms can be given names similar to those of the bridged systems. For example, the system



could be called spiro[3,0,3,2] decane, the figures denoting the numbers of members in the bridges between spiro atoms, in the order in which the "Rules for Numbering" number the system. The number of figures in the brackets is equal to twice the number of spiro atoms present. Perhaps it would be better to say bi- (or di-) spiro[3,0,3,2] decane in the above case and trispiro- when three spiro atoms are present, and thus make the names still more analogous to those of the Baeyer compounds.²² An advantage of using simply spiro- in all cases is that these compounds will then all be found in one place in indexes (as may be seen in the indexes to *Chemical Abstracts*).

²¹ Such indices were proposed by Buchner and Weigand, *Ber.*, **46**, 2110–2113 (1913). They are here used in a slightly different and (the writer believes) clearer manner.

²² See Radulescu, Ber., 44, 1023-1024 (1911).

Hetero atoms may be indicated in the same way as recommended for bridged systems. Thus, the system



would be called spiro[2,4]diaza-1,3-heptene-2 (or -hepten-2-ine).

Complex Spiro Systems (Class D II)

These systems contain other unions in addition to the spiro unions and are numbered provisionally in the "Rules for Numbering." They may be given corresponding names by juxtaposing the names of the components after the prefix "spiro" and indicating which is the common atom. For example, the system



would be spiro-bicyclo(2,1,0)pentane[5,1']cyclohexane, while the unusually complex system



would be spiro-acenaphthene [1,2'] bicyclo(1,1,0) diaza-1',3'-butane [2,3'']-hydrazimethylene. If such a compound should prove of importance as a parent substance a special name should be coined for it, as has been done for fluoran.

Additional References

Beesley and Thorpe, J. Chem. Soc., 117, 591-598 (1920); Béhal, Bull. soc. chim., [4] 11, 264-275 (1912); Beilstein, "Handbuch," 3d ed., Vol. 4, pp. 1-2 (1899); Borsche, Ann., 377, 71-78 (1910); Bredt, Ann., 292, 123 (1896); Bredt and Savelsberg, J. prakt. Chem., 97, 1-22 (1918); Grignard, Chem.-Ztg., 34, 941 (1911); Bull. soc. chim., [4] 11, 124 (1912); Richter, Ber., 29, 586-608 (1896); Stelzner and Kuh, Literatur-Register der organischen Chemie, 3, 13-100 (1921).

Summary

Several general principles are formulated for the correct naming of parent ring systems. The individual classes of ring systems are then considered. The present state of their nomenclature is presented, the more promising methods for forming their names are discussed, and some new proposals are submitted.

Yellow Springs, Ohio