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Graph-Based Chemical Nomenclature. 2. Incorporation of Graph-Theoretical Principles into Taylor's Nomenclature Proposal

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The Taylor nomenclature proposal for organic ring systems is shown to be a suitable starting point for the development of a comprehensive nomenclature system. Changing the basis of the proposal from hydrocarbons to chemical structure graphs permits its extension to other ring systems such as coordination ring systems and boron cages. Addition of a compatible system for acyclic structures will complete the graph-theoretical basis for a comprehensive system.

1. INTRODUCTION

The desire to improve existing nomenclature practices, especially as they relate to indexing purposes, has recently been reviewed.[1] Efforts to improve existing practices have been of two types: (1) codification and systematization of existing nomenclature systems, and (2) proposal of new systems. Because proposed systems[2-9] have been limited in scope, they therefore have also been of limited practical value for general indexing purposes. Potentially the most successful approach to devising a novel, comprehensive, practical nomenclature system is by incorporation of graph theoretical principles.

Such an approach permits the naming of chemical substances to be divided into three independent steps: (1) numbering and naming the graph, (2) identification of skeletal atoms and bonds, and (3) incorporation of nonskeletal information (e.g., stereochemistry, charges). Since the three steps are independent of each other, only the first step will be discussed here as part of an effort to determine the best procedure for numbering and naming graphs; the remaining steps will be discussed in subsequent papers in the series.

The first comprehensive nomenclature system to be based on chemical structure graphs was proposed by Lozac'h et al.[10] Nodal nomenclature, as it is called, is itself a development of von Baeyer nomenclature[11] in which a ring system is numbered by choosing a path through it. An alternative method of numbering a ring system, proposed by Taylor[2] and discussed here, is to number each component ring in turn.

It is a relatively simple matter to change the base of Taylor's proposal (or, indeed, of any hydrocarbon-based nomenclature system) from hydrocarbons to chemical structure graphs. The

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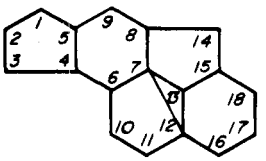

Figure 1. 7(12)-Tria-1,6,8(13)-ternipenta-4,12(15)-binihexalane.

main effects of this change are (1) that valency (or connectivity) of any atom no longer has an upper limit of 4, and (2) that hydrocarbon names can no longer be used as index "parent" names for other chemical structures. The latter effect requires that another source of "parent" names be found.

2. DISCUSSION

Taylor[2] observed that "in the field of ring structures there is no written word or speech equivalent of the structureal formula–names must be associated with the structural formulas by sight". For example, there is nothing in the names "pyridazine", "pyrimidine", and "pyrazine" to indicate that they are the 1,2-, 1,3-, and 1,4-diaza analogs, respectively, of benzene. Taylor therefore attempted to develop "a nomenclature that is integrated with classification". His Latin–Greek combination names are written word or speech equivalents of structural formulas in that they express the number and size of the constituent rings and are, in fact, a verbal form of what is known either as the smallest set of smallest rings (SSSR)[12,13] or as the ring size part of ring analysis[14]. Thus, while 7-(12)-tria-1,6,8(13)-ternipenta-4,12(15)-binihexalane is an unfamiliar name, it does provide a direct correlation between the SSSR of a ring system and its name. It is readily apparent from the name that the ring system is saturated and contains one three-membered, three five-membered, and two six-membered rings. The locant prefixes define the ring system further as that illustrated in Figure 1. Conversely, a saturated ring system with ring sizes 5,5,6,6,6,8 would readily be given the partial name binipenta-ternihexa-octalane, the name being completed by addition of appropriate locant prefixes.

This feature of Taylor nomenclature lends itself directly to both manual and machine manipulation. Coupled with machine methods for determining SSSR,[12,13] it raises the possibility of at least partial name assignment by computer.

Before this can be accomplished, however, some irregularities in Taylor's choice of distributive prefixes (see Table I), no doubt reflecting their Latin origins, must be removed. For example, undeni (one-and-ten) is eleven, but undetriceni (one-from-thirty) is twenty-nine; duodeni (two-and-ten) is twelve, but duotriceni (or duodetriceni?) (two-from-thirty) is twenty-eight. In addition, the teens are reversed with respect to other numbers; e.g., quinideni (five-and-ten) is fifteen but viceniquini (twenty-and-five) is twenty-five. The early multiples of ten are irregular: deni for ten, viceni for twenty, triceni for thirty, then quadrageni for forty, etc.

Dyson and Patterson[7] resolved one problem by proposing octonideni and novenideni for eighteen and nineteen, respectively. However, this problem can be resolved completely by adopting distributive prefixes that parallel the mathematical system of numbering.[15] To do so would require prefixes for the numbers 1 through 9 and for 10, 100, etc. The prefixes used by Taylor for 1 through 9 and for 100 can be retained. Geni is better than deni for 10 because it coincides with Taylor's system above 30 and, more importantly, it avoids ambiguity where senideni represents 16 in Taylor's system but would represent 60 here. The modified distributive prefixes are illustrated in Table II, from which any distributive prefix from 2 to 199 can be derived (see Table I).

Similar remarks apply to Taylor's Greek number names used to specify ring sizes (Table III). The names are more consistent than the Latin prefixes, the only variation occurring

Table I. Vocabulary for Enumerative Nomenclature: Latin Distributive Prefixes

no. of rings	Taylor's Latin distributive prefix used to designate plurality of rings of each size	modified distributive prefixes
1	singuli[16]	singuli[16]
2	bini	bini
3	terni	terni
4	quaterni	quaterni
5	quini	quini
6	seni	seni
7	septeni	septeni
8	octoni	octoni
9	noveni	noveni
10	deni	geni
11	undeni	genisinguli
12	duodeni	genibini
13	ternideni	geniterni
14	quaternideni	geniquaterni
15	quinideni	geniquini
16	senideni	geniseni
17	septenideni	genisepteni
18	duodeviceni	genioctoni
19	undeviceni	geninoveni
20	viceni	binigeni
21	vicenisinguli	binigenisinguli
22	vicenibini	binigenibini
23	viceniterni	binigeniterni
24	viceniquaterni	binigeniquaterni
25	viceniquini	binigeniquini
26	viceniseni	binigeniseni
27	vicenisepteni	binigenisepteni
28	duotriceni	binigenioctoni
29	undetriceni	binigeninoveni
30	triceni	ternigeni
31	tricenisinguli	ternigenisinguli
32	tricenibini	ternigenibini
40	quadrageni	quaternigeni
50	quinquageni	quinigeni
60	sexageni	senigeni
70	septageni	septenigeni
80	octogeni	octonigeni
90	nonageni	novenigeni
100	centeni	centeni

Table II. Mathematically Derived Distributive Prefixes

100	1–9	10	1–9
centeni	singuli[16]	geni	singuli[17]
	bini		bini
	terni		terni
	quaterni		quaterni
	quini		quini
	seni		seni
	septeni		septeni
	octoni		octoni
	noveni		noveni

in the muiltiples of ten (deca, eicosa,[18] triaconta, tetraconta, etc.) with conta as the preferred term for 10 and addition of hecta for 100. The modified Greek number names are illustrated in Table IV, from which any ring size from 3 to 199 can be derived (see Table III).

It was mentioned above that to change the base of Taylor's proposal from hydrocarbons to graphs means that hydrocarbon names can no longer be used as "parent" names and that another source of such names is needed. The obvious source is the graphs themselves; i.e., the chemical structure graphs need to be named. A term is therefore needed that immediately differentiates between the name of a graph and the name of a chemical structure. In nodal nomenclature,[10] the term is the ending "nodane". Taylor uses the endings "-lane" and "-lene" to represent saturated and unsaturated hydrocarbons, respectively. These terms can be retained with their

Table III. Vocabulary for Enumerative Nomenclature: Greek Number Names

ring sizes	Greek number names used to specify each ring size	modified Greek number names
1	no ring	no ring
2	no ring	no ring
3	tria	tri
4	tetra	tetra
5	penta	penta
6	hexa	hexa
7	hepta	hepta
8	octa	octa
9	nona	nona
10	deca	conta
11	hendeca	contamono
12	dodeca	contadi
13	trideca	contatri
14	tetradeca	contatetra
15	pentadeca	contapenta
16	hexadeca	contahexa
17	heptadeca	contahepta
18	octadeca	contaocta
19	nonadeca	contanona
20	eicosa[18]	diconta
21	hencosa	dicontamono
22	docosa	dicontadi
23	tricosa	dicontatri
24	tetracosa	dicontatetra
25	pentacosa	dicontapenta
26	hexacosa	dicontahexa
27	heptacosa	dicontahepta
28	octacosa	dicontaocta
29	nonacosa	dicontanona
30	triaconta	triconta
31	hentriaconta	tricontamono
32	dotriaconta	tricontadi
40	tetraconta	tetraconta
50	pentaconta	pentaconta
60	hexaconta	hexaconta
70	heptaconta	heptaconta
80	octaconta	octaconta
90	nonaconta	nonaconta
100	_	hecta

Table IV. Mathematically Derived Greek Number Names

100	1-9	10	1-9
hecta	mono[16]	conta	mono[19]
	di		di[19]
	tri		tri
	tetra		tetra
	penta		penta
	hexa		hexa
	hepta		hepta
	octa		octa
	nona		nona

defined meanings and can be differentiated from the corresponding graphs by use of the ending "-gon", which is derived from the Greek γονια, meaning angle or corner. Use of this ending would result in names that are easily recognizable. For example, Taylor's names for benzene and cyclohexane are hexalene and hexalane, respectively. The name of the corresponding graph would be hexagon. Similarly, the graph of the structure illustrated in Figure 1 would be named 7-(12)-tria-1,6,8(13)-ternipenta-4,12(15)-binihexagon.

A ring system such as this is numbered by first selecting an end ring (in this example, a five-membered ring). The system is then oriented with the end (five-membered) ring to the left. The end ring is numbered by assigning locant 1 to a position adjacent to a ring fusion, continuing with the unshared members (locants 2 and 3), and finishing with the ring junctions (locants 4 and 5). Locants (6–9) are then assigned to the unnumbered members of the second (i.e., six-membered) ring with the lowest locant (i.e., 6) being assigned to the position adjacent to the ring junction previously assigned the lower locant (i.e., 4). The remaining locants are similarly assigned to the rest of the ring system in such a way as to yield the lowest numeral prefixes in the name. When a ring is closed to a position whose locant is not one greater than the position to which the addendum is attached, the higher locant is enclosed in parentheses in the name and placed immediately after the lower locant.

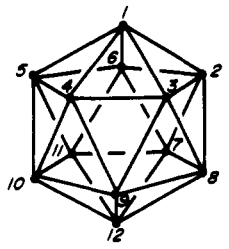

Figure 2. 1,1(3),1(4),1(5),2(6),2(6),2(7),3(8),3(8),4(9),4(9),5-(10),5(10),6(11),7(11),7(11),8(12),9(12),10(12)-Geninovenitrigon.

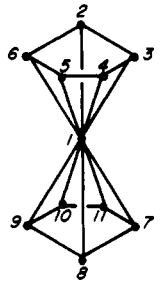

Figure 3. 1,1(3),1(4),1(5),1(1),1(8),1(9),1(10),2(6),7(11)-Genitrigon.

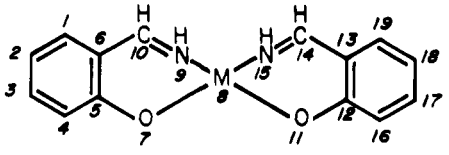

Figure 4. 9,15-Diaza-8-(metal)-7,11-dioxa-8-spiro-1,5,8(8),12-quaternihexalene.

When a structure is drawn from the name, the numeral prefix 1 indicates the first ring to be drawn. In this example, the first ring is a five-membered ring and it is numbered counterclockwise beginning at the top of the ring. The next higher numeral prefix in the name is 4 which indicates, in this example, that a six-membered ring is fused to positions 4 and 5 of the first ring. This is followed, in turn, by a five-membered ring fused to positions 6 and 7, a three-membered ring fused to positions 7 and 12, a five-membered ring fused to positions 8 and 13, and a six-membered ring fused to positions 12 and 15. If the name ends in "-lane", the ring system is a saturated hydrocarbon; if it ends in "-lene", the ring system is an unsaturated hydrocarbon; while if it ends in "-gon", the ring system is a graph.

It was also mentioned above that to change the base of Taylor's proposal from hydrocarbons to graphs means that valency (or connectivity) of any atom no longer has an upper limit of 4. This means that application of Taylor terminology can be extended to include ring systems such as boron cages and metallocenes. Boron cages, such as the icosahedral dodecaboron cage, can be named quite readily by Taylor terminology although the name of the corresponding graph (Figure 2) is longer than the current name of a boron hydride derivative of that structure, such as 1,2-dicarbadodecaborane(12).

However, "dodecaborane(12)" is a name which, as Taylor pointed out, has the disadvantage of having to be associated

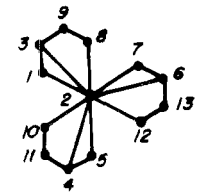

Figure 5. 1,2(2),2(2)-Ternitri-2,2(4),2(6)-ternitetragon.

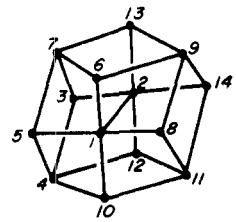

Figure 6. 1(5),1(6),1(8),2(4),3(7),2(7),4(10),9(13),2(9),11,11-(14)-Denisingulitetra-1-pentagon.

with the structural formula by sight. Metallocenes can be named similarly, as illustrated in Figure 3.

Taylor included metal complexes in his proposal, one of which (Figure 4) is a spiro system. It is of interest to note that the term spiro is redundant in Taylor's proposal, because a spiro atom is indicated by a repeated locant (8(8) in the case of Figure 4). The term spiro need not therefore be retained unless it is useful for indexing purposes.

Incorporation of graph theoretical principles into Taylor's proposal permits the numbering and naming of metal complexes of the type illustrated in Figure 5. They can be treated similarly to spiro structures, the repeated locant (in this case, 2(2)) appearing more than once.

Deletion of the spiro class would reduce by one Taylor's six classes of ring systems, viz., Class I, Simple Systems (i.e., single rings); Class II, Unifilar Systems (i.e., unbranched ortho-fused systems); Class III, Polyfilar Systems (i.e., branched ortho-fused systems); Class IV, Spiro Systems; Class V, Reticular Systems (i.e., peri-fused systems); and Class VI, Bridged Systems. However, Taylor did not include a class where every atom (or node) is a bridgehead (i.e., every atom (or node) is common to three or more rings), so there is a need to add a class for those ring systems. It is advantageous to avoid the rather loose term "cage" for this class of ring systems so "fisular" (from the Greek $\phi\nu\sigma\alpha\lambda(\lambda)\iota\varsigma$, meaning bubble) is preferable. The simplest structure of this class is the tetrahedron (e.g., tetraarsatricyclo[1.1.0.$0^{2,4}$]butane), and other members include the cube (e.g., pentacyclo[4.2.0.$0^{2,5}$.$0^{4,7}$]octane) and the icosahedron (e.g., 1,2-dicarbadodecaborane(12)).

Taylor's classification of ring systems into increasingly complex classes, with the more complex class taking precedence over the less complex, is of value when introducing the system. However, for the routine naming of ring systems it is more practical to reverse the classification, with the more complex (and senior) ring systems appearing first. The six classes of ring systems then become, in order of decreasing seniority: Class I, Fisular Systems; Class II, Bridged Systems; Class III, Reticular Systems; Class IV, Polyfilar Systems; Class V, Unifilar Systems; and Class IV, Simple Systems.

Taylor stated that the Greek number names are arranged in order of increasing ring sizes, but made no comparable statement about locant prefixes. In general, the locant prefixes preceding each ring size fall naturally into ascending numerical order. However, in some cases they do not, as in Figure 6. Although the locants are not in ascending numerical order, each ring closure follows naturally the preceding construction steps. If the locant prefixes are arranged in ascending numerical order (i.e., if the name becomes 1(5),1(6),1(8),2-(4),2(7),2(9),3(7),4(10),9(13),11,11(14)-denisingulitetra-1-

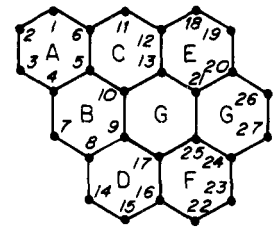

Figure 7. 1,4,6(10),8,12,16,21(25),20(24)-Octonihexagon.

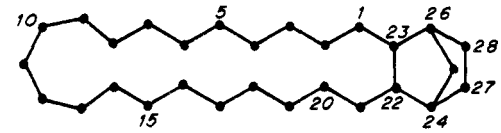

Figure 8. 22,24(26)-Binipenta-1-dicontatrigon.

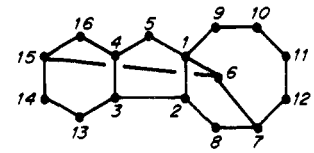

Figure 9. 1,1(2)-Binipenta-3,6(15)-binihexa-1(7)-heptagon.

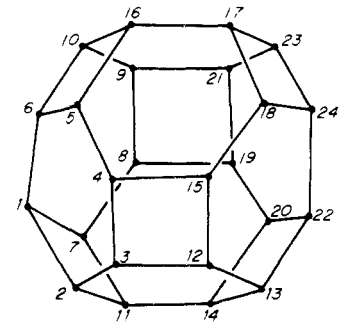

Figure 10. 2(7),4(12),9(19),10(16),13(20),18(23)-Senitetra-1,1-(6),3(11),5(15),8(14),17(21),22(24)-septenihexagon.

pentagon), problems begin to arise at ring closure 2(7). For this reason, it is preferable that the locant prefixes be cited in the sequence required for construction of the ring system.

A similar situation occurs in numbering the graph of benzo[*bc*]coronene. Taylor used coronene as an example, but using the same numbering method for the benzo derivative results in a ten-membered ring that must be divided to form two six-membered rings (G–G in Figure 7). The problem can be resolved by, again, citing locant prefixes in the sequence required for construction of the ring system, as illustrated in Figure 7.

Taylor's numbering system is inconsistent in that it requires the first ring to be numbered in such a manner as to number the greatest number of unshared members first. Subsequent rings are numbered to yield the lowest numeral prefixes. This inconsistency is particularly apparent if the first ring to be numbered is a macrocycle, as in Figure 8. Dyson and Patterson[7] proposed that numbering should begin at a ring junction. This would provide low numbering for the first ring as well as for the rest of the structure. It is also more appropriate for graph-based nomenclature; since the graph is the first part of a structure to be numbered and named, it follows that the graph should have higher priority in numbering than, say, substituents.

Beginning the numbering at a ring junction removes a deficiency in Taylor's proposal, which does not provide rules for numbering heavily bridged (including fisular) ring systems. These ring systems can be numbered satisfactorily by beginning at a ring junction and preferring lowest locants, as in

Figure 9. Similar procedures can be used for fisular ring systems of more than one ring size. In these ring systems, lowest numbering is obtained if numbering begins with the largest ring, as in Figure 10.

3. SUMMARY

Taylor's admittedly incomplete nomenclature proposal for organic ring systems has been shown to be amenable to improvement and extension. Taylor's Latin distributive prefixes and Greek number names are irregular and have been modified to parallel the mathematical system of numbering. Incorporation of graph theoretical principles into Taylor's proposal has permitted its extension to include ring systems containing atoms of valency (or connectivity) greater than 4; i.e., the modified Taylor nomenclature proposal can name any ring system, including metallocenes and "cages". However, a compatible system for naming acyclic graphs must be added before a comprehensive nomenclature system can be developed and compared with the nodal nomenclature approach of choosing a path in order to determine which is the better basis for a comprehensive graph-based nomenclature system.

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(16) Not used, but added for completeness.
(17) Used only when following a multiple of ten, as in 11, 21, 101, etc.
(18) Icosa is now recommended by IUPAC. See "Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F and H"; IUPAC, Pergamon Press: Oxford, 1979; p 5.
(19) These terms are not used alone because the smallest ring has three sides.

Off-Line Input of Chemical Structures with a Low-Cost Microprocessor-Controlled Semigraphical CRT

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Use of a microprocessor-controlled device with semigraphical CRT, light pen, and keyboard in conjunction with a direct access storage medium facilitates and speeds up the input of structural information.

In an earlier publication[1] we outlined the basic concepts of our computer-based documentation system for company research results CCBF (Computer Processing of Chemical and Biological Facts). The system has been further developed in the meantime to keep pace with progress in computer technology. Experience, gained in the daily use of the system, was evaluated and embodied in a series of system expansions and improvements, which are to be reported in the near future.[2] In addition, the steadily increasing costs of manpower forced us to look for a less time consuming means for the input of chemical and, especially, structural information.

Of the known systems, electronic devices using the RAND tablet, graphical CRT, or TV cameras[3-7] had to be excluded because of their high costs and the lack of on-line access to a corresponding computer in our area. Of the less expensive mechanical devices, even the most advanced chemical teletype[8,9] still had apparent drawbacks which we sought to overcome.

The availability of inexpensive microcomputer modules and the fact that floppy disks can serve as an off-line recording medium as well as a random access storage medium allowed the realization of a practice-oriented system tailored to user suggestions and requirements. As can be seen in Figure 1, the device consists of five functional units: (1) control unit containing a MOS Technology 6502 microprocessor, read-only-memory (ROM) program storage, random-access-memory (RAM) as display and working storage, input-output-control and videocontrol; (2) 12-inch industrial b/w video monitor; (3) light pen with integrated amplifier; (4) teletype keyboard, supplemented by a block of 12 keys, which are frequently required with special symbols (especially bond symbols); (5) dual-device floppy disk storage system (IBM 3740 format).

A general flow diagram of the processing program is given in Figure 2. It should be stressed initially that the device can work in two operating modes: "normal-mode", i.e., light pen active; "text-mode", i.e., light pen inactive. The selected mode is indicated by letters A (from German word *A*us = off) and E (from *E*in = on) behind the displayed command word TXT. After initializing, the working grid is displayed, showing three

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