CROATICA CHEMICA ACTA CCACAA **59** (3) 547—563 (1986)

YU ISSN 0011-1643
CCA-1668 UDC 541
Original Scientific Paper

Advantages of Nodal Numbering for Uniquely Identifying Atoms in Chemical Nomenclature

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Received September 2, 1985

There are situations in chemical nomenclature where duplication of locants creates difficulties (a) in describing modifications to chemical structures, (b) in describing stereochemistry, (c) in identifying isotopically-labeled atoms, and (d) in uniquely identifying atoms for crystallography. Nodal nomenclature is shown to avoid these problems and to simplify such descriptions.

INTRODUCTION

The first concerted international agreements on chemical nomenclature were made in Geneva in 1892[1]. From these agreements has arisen the International Union of Pure and Applied Chemistry (IUPAC), as we know it today. IUPAC has, in general, »confined its efforts to codifying sound practices which already existed«[2]. IUPAC has published a set of internationally-agreed rules of organic chemistry[2]. However, more than one sound practice is sometimes described (e. g., for naming organic compounds containing phosphorus, arsenic, antimony or bismuth) without any indication of which practice is preferred. For practical reasons, indexers of chemical literature, such as Chemical Abstracts Service and Beilstein, must be more selective, i. e. more systematic, than IUPAC and must even develop their own rules when IUPAC rules are vague or non-existent.

The rules published by IUPAC include the powerful and commonly-used technique of substitutive nomenclature. In principle, when naming a compound, as large a »parent« as possible is chosen, preferably containing a functional group (e. g., a carboxylic acid). The groups comprising the rest of the molecule are then described as replacements of hydrogen atoms of the parent, i. e., as substituents.

One major problem with the general use of substitutive nomenclature occurs when duplication of locants creates difficulties in describing modifications to chemical structures in describing stereochemistry, in identifying isotopically-labeled atoms, and in uniquely identifying atoms for crystallography.

NODAL NOMENCLATURE

While it can be argued that the percentage of names involved in these difficulties is relatively small, nevertheless the difficulties can be quite severe for some names, particularly when a name is being translated into a structure. These problems can be resolved by use of nomenclature systems that provide unique locants. A particularly fruitful source of such nomenclatures is graph theory, which not only yields unique locants but also provides a mathematical description of the graphs (3).

One such nomenclature is nodal nomenclature, which is comprehensive and incorporates many of the sound practices published by IUPAC. It goes one step further than Chemical Abstracts Service and Beilstein in eliminating ambiguities and in making chemical nomenclature more systematic. In particular, use of the substitutive method is more restricted than before. Nodal nomenclature also incorporates some graph theoretical principles to provide unique numbering of nodes and atoms. While the procedure by which nodal names are generated has already been described[4,5] it would be useful here to review the procedure briefly so that nodal names can be compared with IUPAC names more readily.

As shown in Figure 1, the first step is to ignore all atom and bond identities to yield a graph of nodes and lines. In this example, the carbonyl oxygen atoms and hydroxy groups (including those of the carboxylic acid group) are regarded as substituents[5] and are therefore ignored, together with the hydrogen atoms. The carbon atoms of the carboxy, hydroxymethyl and methyl groups are regarded as part of the skeleton, as are the heterocyclic nitrogen atoms.

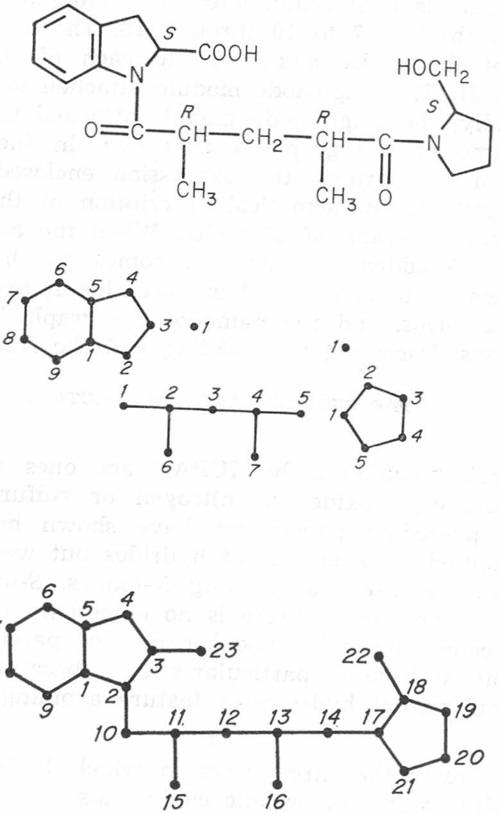
The graph is then broken into cyclic and acyclic modules and each module is numbered in isolation from all other modules; in other words, the numbering of each module begins with 1.

The modules are then ranked in order of seniority according to the following criteria[4], which are applied successively until a decision is reached:

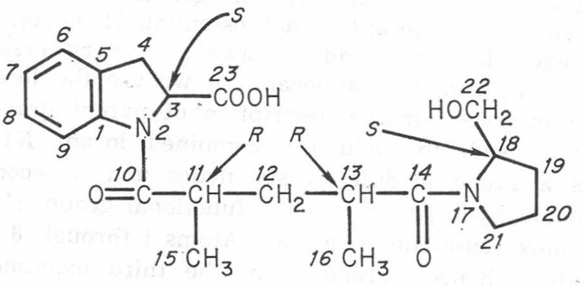
a) Largest number of nodes.
b) Cyclic module preferred to acyclic module.
c) Largest number of rings or branches (side chains).
d) Largest main ring or longest chain.
e) Longest bridge or branch (side chain).
f) Lowest locants for attachment of bridges or branches (side chains).

The most senior module in this example is therefore the one containing the largest number of nodes: it has a ring of nine atoms with a direct bond between nodes 1 and 5 and it retains its original numbering of 1 through 9.

The longest chain of modules (both cyclic and acyclic) takes us through the second most senior module, an acyclic module of seven nodes. There is an unbranched main chain of five nodes, with single-node branches at nodes



Tricyclo[(09.0^{1,5})2:10(5.1^{2}1^{4})14:17(05)18:22(1)3:23(1)] tricosanodane



(3*S*,11*R*,13*R*,18*S*)-22-Hydroxy-10,14-dioxo-2,17-diazatricyclo⊂

[(09.0^{1,5})2:10(5.1^{2}1^{4})14:17(05)18:22(1)3:23(1)] tricosan⊂

(1,5-9)aren-23-oic acid

Figure 1. Derivation of a nodal name.

2 and 4. This module is now renumbered by adding 9 to each locant and changing locants 1 through 7 to 10 through 16. The cyclic module of five nodes is now renumbered by adding 16 to each of its locants, yielding locants 17 through 21. The singlenode module attached to node 18 is renumbered 22 and, finally, the single-node module attached to node 3 is renumbered 23. The name of the graph is as shown in the figure, »tricyclo« implying a total of three rings, the expression enclosed in brackets (i. e., the descriptor) being the mathematical description of the graph, and »tricosanodane« implying a graph of 23 nodes. When the atom, bond, and stereochemical data are added, the name becomes as shown in the figure with the stereochemical data, enclosed in parentheses, preceding substitution terms, replacement terms, and the name of the graph. The term »nodane« is replaced by terms describing the bonding and the functional group.

THE PROBLEM AND ITS SOLUTION

1. *Oxides*

Among the rules published by IUPAC are ones describing modified chemical structures, e. g., oxides of nitrogen or sulfur atoms in organic compounds. In a preceding paper^5, we have shown how the substitutive method can be applied to nodal parent hydrides but we made no reference to the additive method used for naming *N*-oxides, *S*-oxides, *N*-sulfides or similar structures. Nevertheless, there is no objection to using this additive nomenclature in connection with nodal names of parent hydrides. Use of additive nomenclature here is particularly easy because of the sequential numbering of nodal parent hydrides, a feature avoiding any duplication of locants.

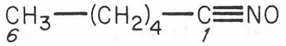
Figure 2. illustrates the three ways in which IUPAC describes oxides of nitrogen or sulfur atoms in organic compounds:

(a) Without Locants — In each example, the IUPAC name relies on there being only one atom to which the term »oxide« can apply. The nodal name of the first example describes an unbranched chain of six atoms and a nitrilo substituent at position 1. Since the nitrogen is the only atom to which the oxide term can refer, a locant is not essential. However, as we prefer redundancies to exceptions, we add a locant in every case. The nitrilo nitrogen does not have a numerical locant, so we use the locant *N*. Superscript locants are reserved for the description of parent graphs, so on-line locants are used instead, to yield the combined locant *N*1. The second example contains a cyclic module of six nodes and a second module of one node. The thioaldehyde group is not a functional group in nodal nomenclature but is a thioxo substituent instead. Atoms i through 6 are connected by aromatic bonding (hence, »arene««). In the third example, locants are again not essential, but are added to avoid exceptions to the rule.

(b) With Element Symbol Locants. — Note that use of the locant in this IUPAC example is inconsistent with earlier acyclic examples, since there is only one atom to which the term »oxide« can apply. The nodal name is simpler because a numerical locant can be used instead of an element

$CH_3-(CH_2)_4-C\equiv NO$

IUPAC : Hexanenitrile oxide

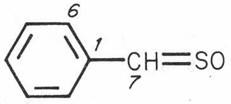


$\underset{6}{C}H_3-(CH_2)_4-\underset{1}{C}\equiv NO$

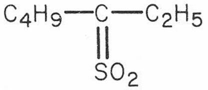
Nodal : 1-Nitrilo[6]hexane *N*1-oxide

$C_6H_5-CH=SO$

IUPAC : Thiobenzaldehyde oxide

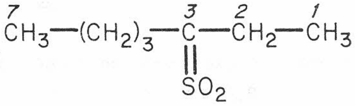


Nodal : 7-Thioxocyclo[(06)1:7(1)]heptan(1-6)arene *S*7-oxide



$C_4H_9-\underset{\underset{SO_2}{\|}}{C}-C_2H_5$

IUPAC : 3-Heptanethione dioxide



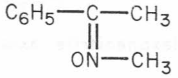
$\overset{7}{C}H_3-(CH_2)_3-\underset{\underset{SO_2}{\|}}{\overset{3}{C}}-\overset{2}{C}H_2-\overset{1}{C}H_3$

Nodal : 3-Thioxo[7]heptane *S*3,*S*3-dioxide

Figure 2a

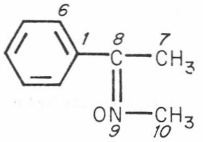
(c) With Numerical Locants. — The IUPAC name of the first example has numerical locants though, strictly speaking, they are not necessary since there is only one atom to which the term »oxide« can apply. The nodal name also has numerical locants because, as before, redundancies are preferred to exceptions. Use of a locant with the oxide term in both names of the second example avoids confusion with incompletely-described compounds.

While these examples explain clearly the principles recommended by IUPAC, they do not provide any guidance on how to avoid ambiguity when naming more complex structures containing more than one nitrogen or sulfur atom. This ambiguity arises from the fact that locants in both the parent and the substituents begin with 1 and thus some locants are duplicated. For example, the structure shown in Figure 3 contains a cyclohexadiene ring and a hexyl chain, each with locants 1 through 6, and an ethyl group with locants 1 and 2. When the imino nitrogen is converted to an *N*-oxide, and



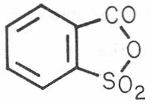
$$\begin{array}{l}C_6H_5-C-CH_3\\ \qquad\ \ \|\\ \qquad ON-CH_3\end{array}$$

IUPAC: *N*-(α-Methylbenzylidene)methylamine *N*-oxide

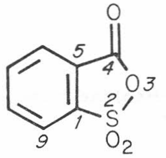


Nodal: 9-Azacyclo[(06)1:8(4)]decan(1-6)aren-8-ene
9-oxide

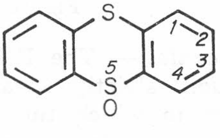
Figure 2b



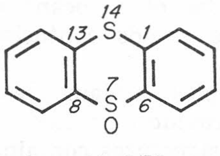
IUPAC: 2,1-Benzoxathiol-3-one 1,1-dioxide



Nodal: 4-Oxo-4*H*-3-oxa-2-thiabicyclo$[09.0^{1,5}]$nonarene
2,2-dioxide



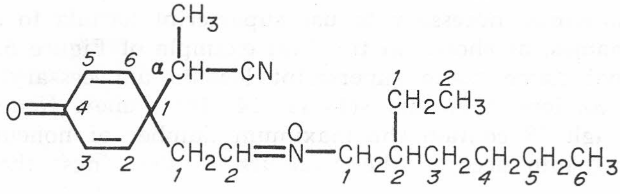
IUPAC: Thianthrene 5-oxide



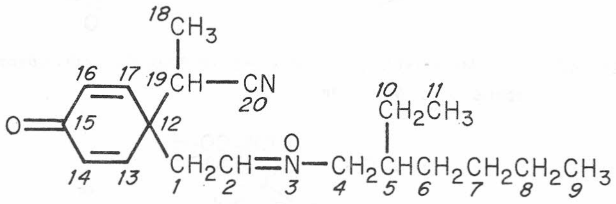
Nodal: 7,14-Dithiatricyclo$[014.0^{1,6}0^{8,13}]$tetradecarene
7-oxide

Figure 2c
Nomenclature of organic oxides. Without locants, Element symbol locants, Numerical locant.

»*N*-oxide« is added after the name, then the question arises: to which nitrogen does the term refer? This ambiguity is removed in the nodal name because the unique numbering permits the use of a numerical locant, in this case, 3-oxide.



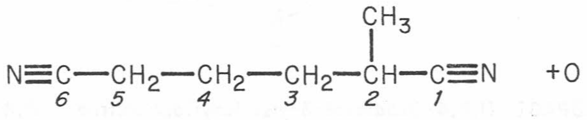
IUPAC: 1-[2-[(2-Ethylhexyl)imino] ethyl]-α-methyl-4-oxo-2,5-cyclohexadiene-1-acetonitrile *N*-oxide



Nodal: 15-Oxo-20-nitrilo-3-azacyclo[(9.2^5)1:12(06)12:19(3)]icosane-2,13,16-triene 3-oxide

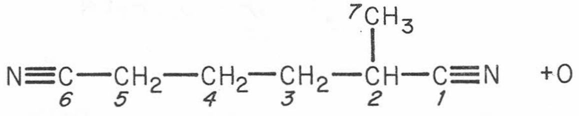
Figure 3. Ambiguity caused by multiple nitrogen atoms.

It is possible to say that no other locant is needed when the nitrile nitrogen is oxidized (as in hexanenitrile oxide, mentioned previously), but that could cause confusion with incompletely-described compounds, where it is not known which nitrogen is oxidized. This is illustrated in Figure 4.



$$N{\equiv}\underset{6}{C}{-}\underset{5}{CH_2}{-}\underset{4}{CH_2}{-}\underset{3}{CH_2}{-}\underset{2}{\overset{CH_3}{CH}}{-}\underset{1}{C}{\equiv}N \quad +O$$

IUPAC: 2-Methylhexanedinitrile oxide



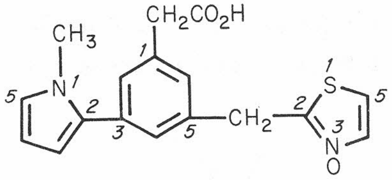
$$N{\equiv}\underset{6}{C}{-}\underset{5}{CH_2}{-}\underset{4}{CH_2}{-}\underset{3}{CH_2}{-}\underset{2}{\overset{^{7}CH_3}{CH}}{-}\underset{1}{C}{\equiv}N \quad +O$$

Nodal: 1,6-Dinitrilo[6.1^2]heptane monooxide

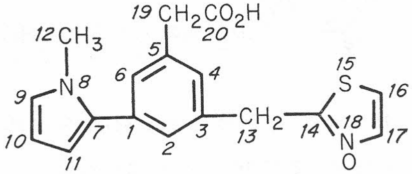
Figure 4. Incompletely-described compounds.

The IUPAC name for this example is ambiguous because »oxide« could also imply the dioxide. The use of a Greek multiplying prefix, such as »mono«, adds some specificity to the names of such incompletely-described compounds. This has been done in the nodal name, but »monooxide« would be preferable for both names.

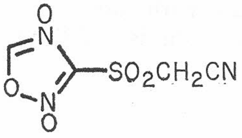
It is sometimes necessary to use superscript locants to avoid ambiguity in IUPAC names, as shown in the first example of Figure 5. Unique locants for the nodal name make superscript locants unnecessary. Note here the use of the condensed locants »(1—11, 14—18) arene«. Nodes 1 through 11 and 14 through 18 contain the maximum number of noncumulative double bonds, taking into account the structure of the rings: the nitrogen atom



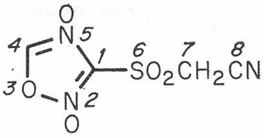
IUPAC: 3-(1-Methyl-1H-pyrrol-2-yl)-5-(2-thiazolylmethyl)benzene ⊂
acetic acid N^3-oxide



Nodal: 15-Thia-8,18-diazatricyclo[(06)1:7(05)8:12(1)3:13(1) ⊂
13:14(05)5:19(2)]icosan(1-11,14-18)aren-20-oic acid
18-oxide



IUPAC: (1,2,4-Oxadiazol-3-ylsulfonyl)acetonitrile N,N'-dioxide

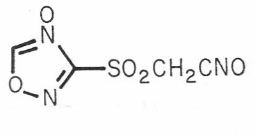


Nodal: 8-Nitrilo-3-oxa-6-thia-2,5-diazacyclo[(05)1:6(3)] ⊂
octan(1-5)arene 2,5,6,6-tetraoxide

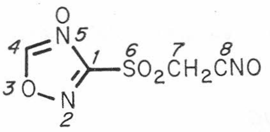
Figure 5. Use of superscript locants and primes.

numbered 8 is substituted and the sulfur atom numbered 15 cannot bear a double bond. Similar remarks apply to the use of primed locants in the IUPAC name of the second example of Figure 5 and to the nodal term »(1—4) arene«.

However, if the nitrile nitrogen is oxidized instead of one of the ring nitrogens, the resulting structure (Figure 6) is difficult to name by IUPAC rules and the name is ambiguous. The nitrile nitrogen is given the locant *N*8 for reasons described above.



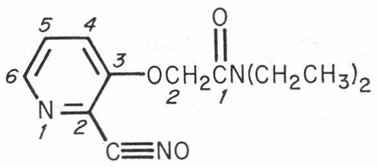
IUPAC: (1,2,4-Oxadiazol-3-ylsulfonyl)acetonitrile dioxide



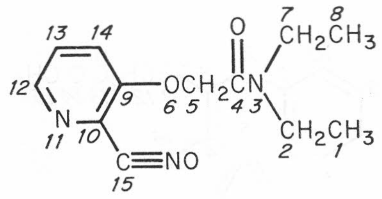
Nodal: 8-Nitrilo-3-oxa-6-thia-2,5-diazacyclo[(05)1:6(3)]⊂
octan(1-5)arene 5,6,6,*N*8-tetraoxide

Figure 6. Loss of information through lack of suitable locants.

Even when superscript locants and primes are used, there is no guarantee that they will provide unambiquous names, as shown in Figure 7. Here, a



IUPAC: 2-[(2-Cyano-3-pyridyl)oxy]-*N*,*N*-diethylacetamide
N^2-oxide



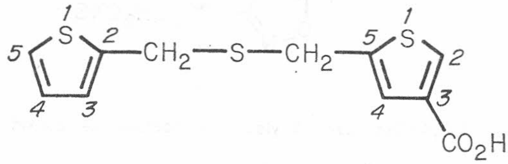
Nodal: 15-Nitrilo-4-oxo-6-oxa-3,11-diazacyclo[(6.2^3)6:9(06)⊂
10:15(1)] pentadecan(9-14)arene *N*15-oxide

Figure 7. Ambiguous superscript locants.

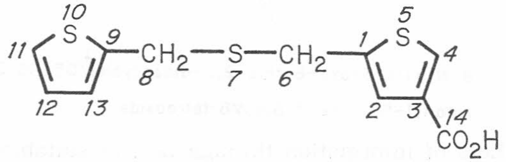
superscript locant is necessary to show that it is the nitrile, not the amide, nitrogen that has been oxidized. However, the locant 2 of N^2 can refer to either the pyridine ring or the acetamide parent. The nodal name remains explicit through use of the locant $N15$.

N-Sulfides are treated similarly to *N*-oxides.

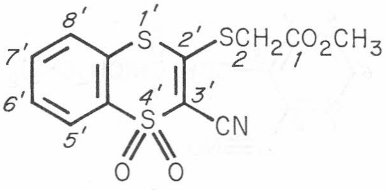
Ambiguity can also arise when describing *S*-oxides, as shown in Figure 8. The first example, with all three sulfur atoms in oxidation state 2, would be named as shown. If the sulfur atom of the parent thiophene ring is



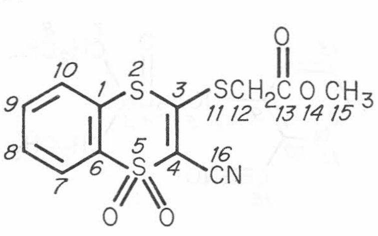
IUPAC: 5-[[(2-Thienylmethyl)thio]methyl]-3-thiophenecarboxylic acid



Nodal: 5,7,10-Trithiabicyclo[(05)1:6(3)8:9(05)3:14(1)]tetradecane-1,3,9(13),11-tetraen-14-oic acid



IUPAC: Methyl 2-[(3′-cyano-1′,4′-benzodithiin-2′-yl)thio]acetate 4′,4′-dioxide



Nodal: 16-Nitrilo-13-oxo-14-oxa-2,5,11-trithiabicyclo[(010.$0^{1,6}$)3:11(5)4:16(1)]hexadecan(1–10)arene 5,5-dioxide

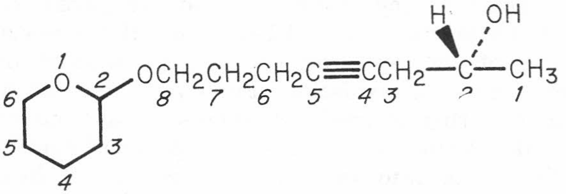
Figure 8. Ambiguity caused by multiple sulfur atoms.

oxidized, the locant of the sulfur atom in the parent can be used to locate the oxygen atoms precisely (i. e., 1,1-dioxide). If the acyclic sulfur is oxidized, then the name of the resulting group (i. e., sulfinyl or sulfonyl) describes precisely the degree of oxidation. Finally, if the sulfur atom of the substituent thiophene ring is oxidized, then we have no choice but to use the term *S,S*-dioxide. While this term is unambiguous here, nevertheless someone translating the name into the structure could not be entirely sure which sulfur atom has been oxidized, although he would know that both oxygen atoms are bonded to the same sulfur atom. If the user understands that the name refers to a precise structure, he has to proceed by elimination of implicit alternatives, arguing that the »dioxide« cannot refer to the parent, because the locants would be 1,1-, and neither can it refer to the acyclic sulfur atom because it would then be named sulfonyl. This type of reasoning is obscure and dangerous because it rests on elimination of supposedly well-defined possibilities and no one can be sure how the user will proceed. Chemical nomenclature must rely, instead, on positive information. For this reason, the structure would be named more precisely by using primed locants (which are uncommon) for the thiophene ring to give 5-[(2'-thienyl)methylthiomethyl]-3-thiophenecarboxylic acid 1',1'-dioxide or by use of the lambda convention to give 5-[[1,1-dioxo-2-(1*H*-1λ^6-thienyl)]methylthiomethyl]-3-thiophenecarboxylic acid. There is no way to define a preferred IUPAC name in this case, which shows that it is probably often safer to speak of »a possible IUPAC name« rather than of »the IUPAC name«. By contrast, in nodal nomenclature, the parent compound always has the same numbering and the three structures would be named simply by adding 5,5-dioxide, 7,7-dioxide, or 10,10-dioxide to the name of the parent compound.

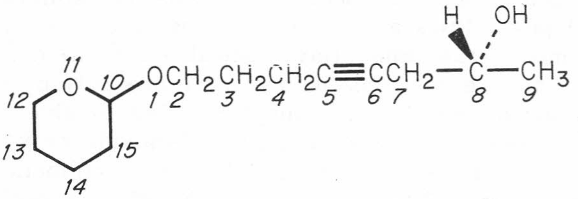
A similar problem exists with the second example of Figure 8. If the acyclic sulfur atom is oxidized, then the IUPAC name of the resulting group (sulfinyl or sulfonyl) is specific. But if a ring sulfur is oxidized, the term would be »oxide« or »dioxide«. These terms are confusing because either could imply an incompletely-described compound with any of the three sulfur atoms or the nitrogen atom being oxidized. When using primed locants for the IUPAC name to avoid this confusion, the lowest possible locant is given to the point of attachment of the heterocyclic substituent. The name is then as shown in the figure. When lambda nomenclature is used, the lowest possible locant is given to the sulfur atom having a non-standard bonding number. The name is then methyl 2-[(2-cyano-1,1-dioxo-1λ^6-1,4-benzodithiin-3-yl)thiolacetate. These problems do not occur with the nodal name.

2. *Stereochemistry*

Duplication of locants can also lead to loss of stereochemical information if no distinction is made between locants, as illustrated in Figure 9. The hydrogen atom at the junction of the ring and side chain is labile, resulting in a racemic mixture. The potential stereochemical center here is therefore routinely ignored and chiral information of any other center is cited as if the racemic center does not exist. A problem arises if another stereochemical center exists at locant 2 of another ring or side chain. When



IUPAC: (2*R*)-8-[(Tetrahydro-2*H*-pyran-2-yl)oxy]-4-octyn-2-ol



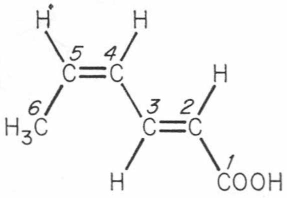
Nodal: (8*R*)-1,11-Dioxacyclo[(9)1:10(06)]pentadecan-5-yn-8-ol

Figure 9. Potential loss of stereochemical information.

this occurs, the locant 2 is ambiguous if no distinction is made. IUPAC avoids this problem by placing the stereochemical information related to the parent in front of the name and other stereochemical information inside parentheses and brackets, as needed. Thus, if it were necessary to cite the stereochemistry at position 2 of the pyran ring, then it would appear immediately in front of »Tetrahydro«. Because of the unique numbering of nodal nomenclature, all of the stereochemical information can be grouped together at the front of the name.

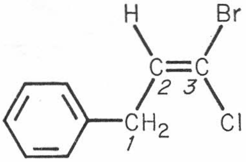
The IUPAC citation of stereochemistry residing in a parent in parentheses in front of the name, is illustrated again with an acyclic structure that is the first example of Figure 10. For simple structures, such as this, IUPAC and nodal stereochemical descriptors can be identical. Strictly speaking, the locant 1 is not essential for the »oic acid« group in the nodal name, but it is included because some redundancy is preferred to exceptions to rules.

Similarly, if a single stereochemical center exists in a substituent, then it, too, is cited before the name, as shown in the second example of Figure 10. Again, the nodal stereochemical descriptor is identical with that of the IUPAC name. Note here use of »axene« in the nodal name to imply a combination of aromatic and other unsaturaion. When a stereochemical center exists in each of two substituents, then the stereochemistry is cited in each substituent name instead of in front of the whole name, as shown

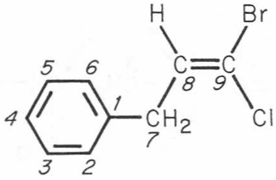


IUPAC: (2*E*,4*Z*)-2,4-Hexadienoic acid

Nodal: (2*E*,4*Z*)-[6]Hexane-2,4-dien-1-oic acid



IUPAC: (*E*)-(3-Bromo-3-chloroallyl)benzene



Nodal: (*E*)-9-Bromo-9-chloro-7*H*-cyclo[(06)1:7(3)]nonaxene

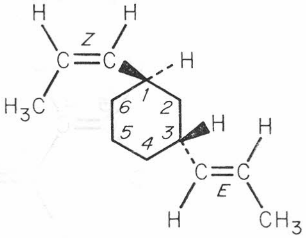
Figure 10. Expression of stereochemistry in the parent and substituent.

in Figure 11. The unique numbering of nodal nomenclature permits collection of the stereochemical terms in one place, at the front of the name.

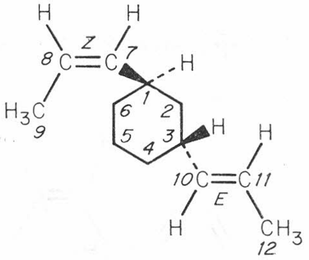
Unfortunately, the IUPAC rules do not contain any moderately complex examples illustrating citation of chirality. Figure 12. illustrates such a structure, in which stereochemistry exists in a substituent which is named as a substituent of another substituent. Here, the stereochemical citations are scattered throughout the name, but nodal nomenclature is able to collect the terms together at the front of the name.

3. *Isotopically-Labeled Compounds*

A similar situation exists for isotopically-labeled compounds. When a parent is isotopically labeled, IUPAC rules require that the description be placed before the name, as shown in the first example in Figure 13. Note that here the IUPAC and nodal names are identical. However, duplication

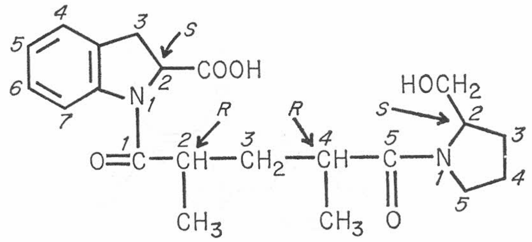


IUPAC: 1-[(*Z*)-1-Propenyl]-*trans*-3-[(*E*)-1-propenyl]cyclohexane

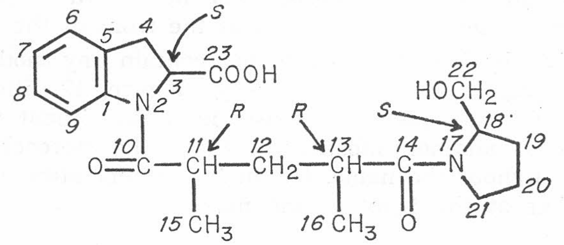


Nodal: (1,3-*trans*,7*Z*,10*E*)-Cyclo[(06)1:7(3)3:10(3)]dodecane-7,10-diene

Figure 11. Expression of stereochemistry in both the parent and substituents.



IUPAC: (2*S*)-1-[5-[(*S*)-2-(Hydroxymethyl)-1-pyrrolidinyl]-(*R*,*R*)-2,4-dimethyl-1,5-dioxopentyl]-2,3-dihydro-1*H*-indole-2-carboxylic acid



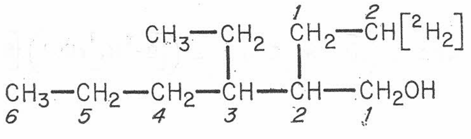
Nodal: (3*S*,11*R*,13*R*,18*S*)-22-Hydroxy-10,14-dioxo-2,17-diazatricyclo[$(09.0^{1,5})$2:10$(5.1^{2}1^{4})$14:17(05)18:22(1)3:23(1)]tricosan(1,5-9)aren-23-oic acid

Figure 12. Expression of stereochemistry of a substituent of a substituent.

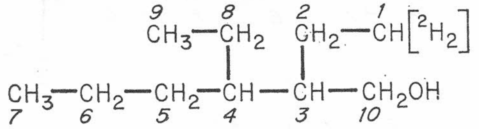
$$CH_2{}^2H—CH^3H—OH$$

IUPAC: $(2\text{-}{}^2H_1,1\text{-}{}^3H_1)$Ethanol

Nodal: $(2\text{-}{}^2H_1,1\text{-}{}^3H_1)$Ethanol



IUPAC: $2\text{-}([2,2\text{-}{}^2H_2]\text{Ethyl})\text{-}3\text{-ethyl-1-hexanol}$



Nodal: $[1,1\text{-}{}^2H_2]\,[7.2^4 1^3]$Decan-10-ol

Figure 13. Expression of isotope data in the parent and substituent.

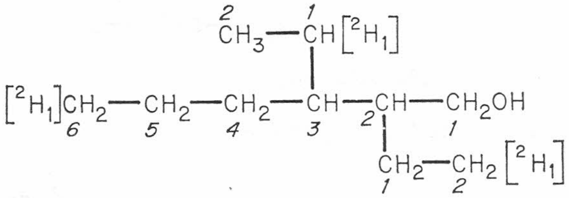
of locants in IUPAC names can require that otherwise identical substituents be treated differently, as in the second example in Figure 13, whereas similar treatment is possible with nodal nomenclature.

Figure 14, illustrates the complexity that can arise when a compound is isotopically labeled in both its substituents and its parent. The description of the labeling is distributed throughout the name in both IUPAC examples, whereas the citation is much simpler in the nodal names.

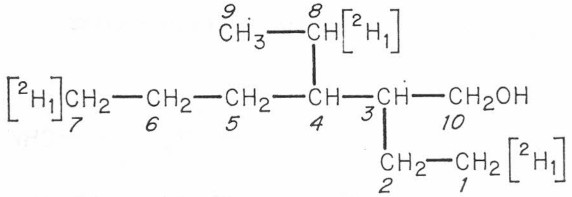
4. *Crystallography*

Crystallographers performing ^{13}C-NMR on a series of related compounds frequently encounter difficulties when attempting to describe the effect of variation in substitution on the spectral properties of a particular atom. Variation in substitution often leads to variation in the names and, hence, the numbering of the particular atom. An example is illustrated in Figure 15.

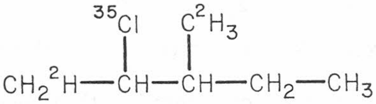
The solution to this problem is for the crystallographers to determine which atoms are common to the structures they are investigating and which atoms are variables. In other words, they construct from a series of related compounds a Markush structure. The Markush structure is then uniquely numbered according to nodal nomenclature principles, as shown in this example. One advantage of nodal nomenclature here is the ability to condense a number of atoms into a supernode, which can be subsequently expanded when needed. For example, each ring or chain in the Markush structure can be drawn to represent the smallest ring or chain in the series of compounds being studied and a unique locant can be assigned to the atom of interest.



IUPAC: 3-([1-$^{2}H_{1}$]Ethyl)-2-([2-$^{2}H_{1}$]ethyl)[6-$^{2}H_{1}$]-1-hexanol



Nodal: [1,7,8-$^{2}H_{3}$][$7.2^{4}1^{3}$]Decan-10-ol



IUPAC: 2-(^{35}Cl)Chloro-3-[($^{2}H_{3}$)methyl](1-$^{2}H_{1}$)pentane

Nodal: 2-(^{35}Cl)Chloro(1,6,6,6-$^{2}H_{4}$)[5.1^{3}]hexane

Figure 14. Expression of isotope data in both parent and substituent.

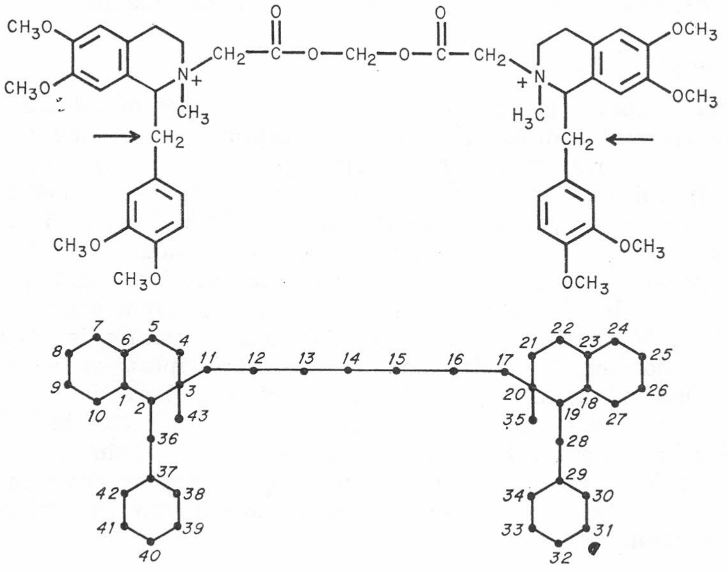


Figure 15. Unique numbering for crystallography.

In this example, the naphthalene and benzene rings remain constant but the substituents on the ring systems can vary in position. They are therefore not included in the graph. The nodes being investigated are indicated by arrows in the figure and are numbered 28 and 36. The nodal name for the Markush graph is Hexacyclo[(010.01,6)3:11(7)17:20(010.01,6)19:28(1)-28:29(06)20:35(1)2:36(1)36:37(06)3:43(1)]tritetracontanodane.

CONCLUSION

We have shown how graph theory can help resolve a number of problems in chemical nomenclature caused by duplication of locants. The unique numbering system described may be of more general use than chemical nomenclature.

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SAŽETAK

Prednosti modalnog označavanja za jedinstveno identificiranje atoma u kemijskoj nomenklaturi.

A. L. Goodson i N. Lozac'h

Sadašnja kemijska nomenklatura ima poteškoća pri opisivanju modifikacija kemijskih struktura, opisa stereokemije, identificiranju izotopski obilježenih atoma i jedinstveno identificiranje atoma u kemijskoj strukturi u kristalografiji. Nodalna nomenklatura nema tih problema i pojednostavnjuje opis kemijskih struktura.