CGNMP 60439-60-3
Spirost-2-eno[2,3-d]isoxazole ([4aS-(4aα,4bβ,6aα,6bβ,7β,8β,9aβ,10aβ,10bα)]-3',4,4',4a,4b,5,5',6,6',6a,6b,7,9a,10,10a,10b,11,12,12a,13-eicosahydro-4a,5',6a,7-tetramethylspiro[8H-furo[2'',3'':4',5']cyclopenta[1',2':7,8]phenanthro[3,2-d]isoxazole-8,2'-[2H]pyran])
$C_{28}H_{41}NO_3$
T H5 F6 E6 B655 JNO UOX&TTTTTJ
B1 F1 W1 V-& BT6OXTJ E1
Text descriptor 4:.SPIROST..7
7 Ring System
5,5,5,6,6,6,6
C_3NO–C_4O–C_5–C_5O–C_6–C_6–C_6
CA 85:78257p

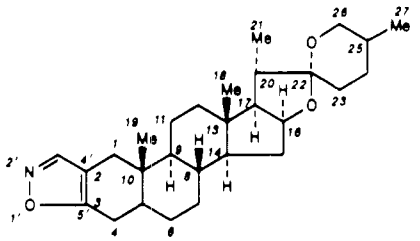

Figure 13. Stereo Parent entry CGNMP.

appear in CA indexes under the name of the acid.

SUMMARY

The PCH has been in use now for more than three years. It contains more than 50 000 entries and serves as a valuable reference tool for those engaged in searching the chemical literature. It is the only complete listing of organic ring systems available. With its periodic updates, it continues to be a complete reference tool. It is especially useful as a current-awareness service for identifying new ring systems, boron cages, metallocenes, and stereoparents.

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(7) See the Introduction to the Ring Analysis Index.
(8) Cyclic substituents are considered a separate ring system and would be treated separately.
(9) Alternatively, the number of rings may be calculated from the formula: no. of rings = no. of edges − no. of atoms + 1 (where the number of edges is the number of distinct atom-to-atom connections). For the ring system of interest, the formula is: 14 edges − 11 atoms + 1 = 4 rings.

Graph-Based Chemical Nomenclature. 1. Historical Background and Discussion

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Events leading to development of chemical nomenclature based on graph theory are described. Chemical nomenclature is defined and distinguished from chemical line notations and connection tables, with which it is sometimes confused. Development of chemical nomenclature from the era of ancient civilizations to the present time is reviewed and the recognized limitations of current practices are described. The case for consideration of a new approach to chemical nomenclature is presented, and the requirements for such a nomenclature to be acceptable to the chemical community are discussed. The development of graph theory and its application to chemistry are reviewed; its advantages as the basis of a single, comprehensive chemical nomenclature are presented.

1. INTRODUCTION

Nomenclature is defined[1a] as: "a system or set of names or designations used in a particular science, discipline, or art and formally adopted or sanctioned by the usage of its practitioners." Chemical nomenclature is more specifically defined as: "a set of chemical names that may be systematic...or not and that aims to tell the composition and often the structure of a given compound by naming the elements, groups, radicals, or ions present and employing suffixes denoting function..., prefixes denoting composition..., configuration prefixes..., operational prefixes..., arabic numbers or Greek letters for indicating structure (as positions of substituents), or Roman numerals for indicating oxidation state." Chemical nomenclature can be illustrated with reference to Figure 1. The substance depicted is named (systematically) 1,4-benzenediol in the *Chemical Abstracts* (CA) Ninth Collective Chemical Substance Index but is more commonly known by its trivial (i.e., nonsystematic) name: hydroquinone.

Nomenclature should not be confused with chemical line notations or connection tables, as sometimes occurs. A notation is defined[1b] as: "a system of characters, symbols, or abbreviated expressions used in...science to express technical facts, quantities or other data". To illustrate a notation, the Wiswesser Line Notation (WLN)[2] for 1,4-benzenediol (hydroquinone) is QR DR. A connection table[3] is "a uniquely ordered list of the node symbols of the structure (or graph) in which the value (atomic symbol) of each node and its attachment (bonding) to the other nodes of the total structure are described." The Chemical Abstracts Service (CAS) Registry III connection table for 1,4-benzenediol is illustrated in Figure 2. Thus, nomenclature, notations, and connection tables are quite distinct from each other and need not be confused.

Nomenclature, notations, and connection tables are of value in different ways. Connection tables are useful as detailed, atom-by-atom computer records of chemical structures, as in the CAS Registry File. Chemical line notations, such as WLN's, are convenient tools for manual or machine registration and substructure searching of files of moderate size (50 000–100 000 structures), although they are used for some

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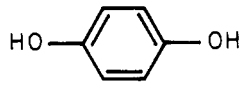

Figure 1.

```
TOPOLOGY

  ATOM NO      1   2
  CONN
  ELEMENT      0   0
  BOND

  RING CORRESPONDENCE LINK

  RING ID              46T.150A.182
  RING ATOM NOS          1   2   3   4   5   6
  SUBSTANCE ATOM NOS   03  04  05  06  07  08

  LINK GROUP      01 -1 03, 02 -1 08

RING

  RING IDENTIFIER NO = 46T.150A.182

  ATOM NO    1   2   3   4   5   6
  CONN       01  01  02  03  04
  ELEMENT    C   C   C   C   C   C

  BOND       *5  *5  *5  *5  *5

  RING CLOSURE PAIRS    05 *5 06
```

Figure 2.

large files (exceeding 1 million structures). Nomenclature is of value for oral and written communication. It has wider application and greater flexibility than chemical line notations and connection tables because substances can be named even if their structures are unknown or are only partially known. Names given to substances of this type cannot be systematic but they can be unambiguous.

Names are the oldest and most common means of access to the chemical literature, e.g., through CA indexes. The terminology used in such indexes must therefore reflect general use and must be at least reasonably familiar to chemists searching the indexes. In the past, trivial names were used extensively for this reason, but more recently it has become less practical to do so and use of trivial names has declined in favor of more systematic names.

While there is still a need for trivial names for incompletely known substances, systematic names are preferable for indexing purposes because names of related substances can be grouped reasonably close together in a highly ordered, sorted index. The structures of the basic component parts can then be illustrated, providing an easy translation of a name to the corresponding chemical "picture".

It is self-evident that, ideally, nomenclature used for indexing purposes should be a single system; should be comprehensive; should not require continual revisions; should have few, simple rules with no exceptions; and, last but not least, should be acceptable to and usable by the chemical community. CAS has cooperated with other organizations for many years to modify existing nomenclature systems in an effort to achieve this goal. However, it appears doubtful that this goal can ever be completely achieved in this manner.

In these and related studies, CAS has explored the possibility of devising entirely new nomenclature systems. One approach involves application of a technique generally known as "graph theory". In the graph of a chemical structure, each atom can be represented by a dot and each bond by a line. A general chemical structure graph can be defined as a set of dots (called nodes), representing unspecified atoms, arranged in a particular pattern and joined by a set of lines, representing unspecified bonds. A graph is a geometrical diagram.

It has not been the objective of these and related studies to design a new system of chemical substance names for immediate use in CAS services. However, we did seek to offer the community a possible alternative, comprehensive system which would not require continual modification. The new system could be made available for the use of the chemical community in addition to existing nomenclature. Whether it will ever replace existing nomenclature in CAS services will depend entirely on its future acceptance and use in the community.

2. DEVELOPMENT OF NOMENCLATURE

The origins of modern nomenclature can be traced back to ancient civilizations when symbols, which are closely related to nomenclature, were used as long ago as in ancient China and Egypt. Their development into modern chemical formulas, notations, and graphs has been reviewed by Rouvray.[4]

Early chemical terminology[5] was concerned primarily with naming inorganic substances, and no logical system based on chemical structures was possible at that time. Names were therefore based on historical association (e.g., Epsom salt for magnesium sulfate), physical properties (e.g., spirit of wine for ethyl alcohol), or physiological behavior (e.g., caustic soda for sodium hydroxide). As evidence of the atomic nature of matter began to accumulate, the need for systematic names based on chemical structures began to be recognized. The first systematic nomenclature proposal to be widely adopted was developed by de Morveau, Lavoisier, Berthollet, and de Fourcroy in 1787.[6]

Although this proposal named a few organic compounds, not enough was known about organic chemistry at that time for difficulties to arise in naming. By 1892, however, organic chemistry was expanding rapidly and the situation was quite different when the International Commission for the Reform of Chemical Nomenclatue met in Geneva.[7,8] Although efforts had been made previously to systematize hydrocarbon names,[9] this was the first time that a concerted international effort had been made to develop coherent policies. Since then, codification and systematization of existing organic nomenclature practices have continued under the auspices of the International Union of Pure and Applied Chemistry (IUPAC).[10] These efforts have been well documented.[11-26]

The first international efforts to develop coherent policies for inorganic chemistry were reported by Delêpine[27] in 1926. But the system proposed for inorganic compounds in 1787 was so successful that, apart from the introduction of the concept of complex (or coordination) compounds,[28] there appeared little need for major changes until about 1940.[29,30] Since that time, reform of existing inorganic chemical nomenclature has been reported extensively.[31-39]

The majority of publications calling for improvement of chemical nomenclature deal only with modifying limited numbers of existing names.[40-52] A few papers have been published which propose complete revision of limited areas of organic nomenclature. For example, the system proposed by Taylor[53] covers organic ring compounds only. The classification and nomenclature system proposed by Balaban and Schleyer[54] is even more restricted, covering only diamond hydrocarbons (polymantanes). Balaban[55,56] has also proposed a similarly restricted system for condensed benzenoid hydrocarbons. While the latter has been extended[57] as a notation to include larger and smaller rings, no provision has been made to modify the names accordingly. Of more general utility is the proposal by Terent'ev et al.[58] which covers name construction, numbering, functional groups, acyclic structures, cyclic structures, labeled compounds, and stereoisomers. But even this proposal is restricted by its being based on hydrocarbons. The authors recognized this restriction in their comment:

> There are, however, classes of compounds which can be reduced only formally to hydrocarbons since their basic element is, in fact, not a hydrocarbon unit. We encounter such cases first of all among organometallic compounds, particularly among the compounds of silicon

and, in part, those of nitrogen and its analogs. A special approach to nomenclature questions is necessary for such compounds, which we call "pseudoorganic".

Continual modification of limited areas of existing chemical nomenclature makes necessary continual modification of existing manual and machine files. A consequence of this approach to improving nomenclature practices is that, in addition to the costs of modifying existing files, retrospective literature searches are made more difficult, time-consuming and, therefore, more expensive because in the course of time a chemical substance may have been given more than one name. Even if the name has not been changed, it is still necessary during a literature search to confirm that it has not.

That there are problems with existing nomenclature has been recognized by Scott,[30] Cahn and Dermer,[38] Taylor,[53] Balaban,[55,56] and Terent'ev et al.[58] Efforts to resolve these problems by modification of existing practices have been discussed by Loening,[5] Verkade,[11-25] Fletcher,[59] and Fernelius et al.[60] An alternative to continual modification of existing practices would be to develop a new, systematic terminology from first principles. This approach has been discussed by Fletcher[59] and Fernelius et al.[60] Fletcher noted that "a multiplicity of nomenclature systems, each with its own set of rules" is undesirable "whereas what is really needed is a simple integrated system applicable to all types of chemical compounds". Fletcher further commented that "tremendous strides have been made in the latter direction during the past two decades" although "it appears unlikely that the present rules will ever become thoroughly systematic". Fletcher concluded that it would be necessary to continue with current practices despite their deficiencies because

> First, there is no practical way to revise and republish the tremendous existing chemical literature; hence chemists would have to learn both old and new nomenclature. Second, the task of converting to a fiducial nomenclature by Chemical Abstracts (Service) and other chemical information processing agencies, both public and private, would be time consuming and costly. Third, unless adopted by Chemical Abstracts (Service) for its Subject Indexes, an entirely new organic nomenclature would probably not be widely accepted and used by the chemical profession.

Fernelius et al.[60] raised similar questions concerning development of a new system of nomenclature and concluded that "whatever the weaknesses of our present schemes, we are pretty much stuck with them". The questions they raised were as follows:

> Can we be sure the new scheme will be sufficiently adaptable to accommodate all the new compounds that are going to be discovered even before the scheme is completely formulated? What are we going to do about the handbooks and indexes which are the entrée to existing knowledge? Do we revise these and reissue them or do we ask all users of the literature to learn the old as well as the new scheme, or do we just forget about what has been done before the year 1NN (New Nomenclature)? What do we do when the new scheme is found to be somewhat inadequate? Start all over again? For all of these, who will pay the bills?

Fletcher and Fernelius have raised a number of valid points which will be discussed in turn. While it is true that there is no way to revise and republish existing chemical literature to accommodate a new systematic nomenclature, the same is also true for current nomenclature. This problem was also encountered when CAS introduced Registry Numbers: substances reported in the literature prior to 1965 have not been assigned Registry Numbers unless they have also been reported since that time. Anyone searching the chemical literature may find it necessary to equate muriatic acid with hydrochloric acid and spirits of hartshorn with ammonia. So chemists already have to learn both old and new nomenclature and, with existing practices, appear doomed to do so indefinitely unless the situation can be stabilized. The task of converting to a new system may be costly, but would it be any more costly in the long run than the current practice of continual modification of limited areas?

Cahn and Dermer[38] considered the implications of introducing a new nomenclature when they stated:

> Over the great complexities and illogicalities of current nomenclature hangs the shadow of the computer; the marshalling of 3–4 million structures and their attendant properties is increasingly admitted to be a computer responsibility. Because computers depend on logic, their use promotes systematic nomenclature. The groups of symbols best suited to computer programs to represent compounds, however, are mostly not names. Thus it does not appear that a computer language will soon displace the often arbitrary and sometimes inconsistent current usage.

Cahn and Dermer are correct that introduction of any new nomenclature cannot be contemplated unless it is capable of manipulation by computer. This subject will be discussed more fully later. The computer also provides the opportunity for any new system to be thoroughly tested before the decision is made whether or not it should be adopted by the chemical community, including publications such as *Chemical Abstracts*.

Nomenclature systems based on well-defined structures such as hydrocarbons[53-56,59] prove inadequate when structures for which they have no model or parent structure are encountered. Ironically, it appears that the less information the parent structures contain the more flexible is the terminology and the more easily it can accommodate novel types of chemical structures. Ideally, any novel nomenclature system should be based on parent structures that indicate merely that two or more unspecified atoms are connected by unspecified bonds; this requirement is satisfied by chemical graphs and will be discussed more fully later. The handbooks and indexes that are the entrée to existing knowledge would be treated no differently than at present, when existing rules are modified. With computer assistance, it should be possible to identify and eliminate any inadequacies before the decision is made whether or not to adopt a systematic nomenclature.

3. REQUIREMENTS FOR A NEW NOMENCLATURE SYSTEM

CAS has cooperated for many years with organizations such as IUPAC in efforts to develop a single, uniform system of nomenclature that would have fewer exceptions and therefore simpler rules than existing systems. During that time, various authors have made a number of proposals[53-58] which have been limited in scope. Should these and similar proposals be adopted for all new classes of compounds, the result would be comparable with current practice; i.e., a workable system would exist but is would not be a simplified, integrated, and comprehensive approach to solving the basic problem already described. The approach to development of a systematic nomenclature that has been adopted by IUPAC and followed by CAS has been the systematization and codification of existing, established nomenclature although, as stated by Fletcher,[59] "it appears unlikely that the present rules will ever become thoroughly systematic".

CAS has recently begun exploring the development from first principles of a systematic, comprehensive nomenclature with a single underlying philosophy. Such a nomenclature system would preferably be anticipatory; i.e., should currently

1*H*-Cyclopenta[*c*]furan-4-carboxylic acid
---,3,3a,6,6a-tetrahydro-5-methoxy-1-methyl-3-oxo-
methyl ester, (1α,3aα,6aα)-(±)-

1*H*-Cyclopenta[*c*]furan-5(3*H*)-one
---, tetrahydro-
cis-

Figure 3.

unknown types of structures be identified (as has happened in the past, for example, with boron hydrides and metallocenes), it should be able to name the novel structures without recourse to specialized, trivial names and without continual modification of the rules. One approach would be to name every chemical structure as a hydrocarbon or as a derivative of a hydrocarbon. This approach and its limitations have been discussed above. A better approach is one in which a structural diagram is replaced by dots (representing unspecified atoms) and lines (representing unspecified bonds) to give a geometrical structure called a graph. In a graph-based system, which would have a single underlying philosophy, chemical substances would be named as modifications of the corresponding graphs.

Read and Milner[61] have described the attributes they would wish to associate with an ideal nomenclature system as follows:

1. The names should be linear character strings, to permit lexicographic ordering.

2. A structural formula should give rise to a unique name.

3. The name should permit the retrieval of the structural formula.

4. The coding process should be simple, and preferably it should be possible for a chemist to code a formula without recourse to a computer.

5. The decoding process should also be simple.

6. The coding process should not depend upon chemical intuition; that is, there should exist an effective algorithm for coding, and computer implementation of this algorithm should be feasible.

7. Names should be brief.

8. Names should be pronounceable.

9. Names should be easily comprehensible to chemists.

To these attributes should be added one that any names to be used for indexing purposes should be capable of being divided into convenient components, i.e., heading parent, substitutents, stereochemistry, and other descriptive terms.

Of Read and Milner's attributes, the ones most difficult to comply with would appear to be attributes of 1 and 7. The need for two units of information to be closely associated (e.g., in a von Baeyer name, the length of a secondary bridge and the locants of the atoms to which it is attached) occurs frequently in nomenclature, and this is generally achieved by use of superscripts. This problem can be resolved by the use of suitable flags in names printed by mechanical printers. While brief names are obviously desirable, they are not compatible with systematic names for complex chemical structures. However, attribute 7 is of less importance in an index, such as the *Chemical Abstracts* Chemical Substance Index, than elsewhere because names are fragmented, as illustrated in Figure 3.

4. DEVELOPMENT OF GRAPH THEORY

The first recorded use of graph theory was the resolution of the Königsberg bridge problem by Euler[62] in 1736. Since then, graph theory has been applied to such diverse subjects as civil and electrical engineering, economics, and distribution networks, and to a variety of chemical subjects.

Graph theory was first applied to a chemical problem by Cayley when he proposed the concept of the tree[63] in 1857 and subsequently applied the concept to enumeration of hydrocarbon isomers[64] in 1874. Since then, graph theory has been applied to a range of chemical subjects such as reaction graphs, synthesis design, chemical documentation, and kinetics. Very little work has been done, however, on application of graph theory to chemical nomenclature.

For the chemist unfamiliar with graph theory, an excellent introduction to the subject is "Chemical Applications of Graph Theory",[57] which covers the history of graph theory, enumeration of isomers, topology, and application of graph theory to organometallic chemistry and polymers. A list of definitions collected by Essam and Fisher[65] provides a useful introduction to the terminology of graph theory.

5. APPLICATION OF GRAPH THEORY TO CHEMICAL NOMENCLATURE

Chemical nomenclature proposals based on hydrocarbons are of limited applicability because they cannot be used directly for chemical structures, such as boron cages and metallocenes, which contain atoms of valency (or connectivity) greater than 4 and for which there are no corresponding hydrocarbons. However, the concepts contained in such proposals can often be extended to graph-based nomenclature.

Conceptually, for both cyclic and acyclic structures, there are two approaches to numbering and naming chemical graphs. For ring systems, the approaches are (i) to pick a path through each ring system, and (ii) to number and name each component ring in turn. For acyclic systems, they are (i) to consider each system as one unit, and (ii) to consider each system as the sum of unbranched components.

Of the nomenclature proposals based on hydrocarbons to which graph theory can be applied, the one developed by von Baeyer[69] encompasses the approach of picking a path through ring systems, with heteroatoms being named by replacement ("a") nomenclature.

Taylor[53] adopted the alternative approach of numbering and naming component rings in his proposal. Again, replacement nomenclature was used for heteroatoms. Taylor's numbering system was subsequently modified by Dyson and Patterson.[67] Fletcher and Butler[68] also modified Taylor's nomenclature system and used it, together with their nomenclature for acyclic structures,[69] for indexing a wide variety of organic compounds. When numbering and naming acyclic structures, Fletcher and Butler regarded each structure as one unit; i.e., the name indicated the total number of atoms in the structure and branching was indicated by locant numbers in brackets before the name.

Perhaps the most comprehensive hydrocarbon-based nomenclature proposal to date is that of Terent'ev et al.[58] in which ring systems are numbered by picking a path, and acyclic compounds are numbered and named as sums of unbranched components.

Of the nomenclature proposals based on graph theory, the one proposed by Balaban[55,56] for condensed benzenoid hydrocarbons greatly reduces the diversity of names for these compounds. For example, pentacene, pentaphene, and picene are named (000)-, (010)-, and (121)pentacatafusene, respectively, the name indicating the number of component (i.e., fused benzene) rings and the numbers how they are arranged within the structure. Balaban has extended this nomenclature

proposal, as a notation only,[57a] to structures containing rings larger or smaller than the benzene ring.

Balaban and Schleyer[54] have applied the principles developed for condensed benzenoid hydrocarbons to propose a nomenclature system for diamond hydrocarbons (polymantanes) that, again, greatly reduces the diversity of names.

The only comprehensive graph-based nomenclature system proposed to date is that developed by Lozac'h et al.[70] and called "nodal nomenclature" from the nodes representing atoms in graphs. This proposal is a development of von Baeyer nomenclature and numbers a ring system by picking a path. An acyclic structure is considered as one unit. Its name indicates the number of atoms; the sizes of any branches and their location are indicated in brackets at the front of the name.

Work on this nomenclature proposal was begun independently by Lozac'h and CAS (in studies related to the present ones) and proceeded jointly from 1975, when it became apparent that the two efforts were proceeding along similar lines. This nomenclature proposal is not limited to organic substances but can also number and name coordination and other structures. In general terms, a chemical structure is named by first deriving the corresponding graph, naming the graph, and then naming the chemical structure as a derivative of the graph. This is the first time that graphs, as opposed to chemical structures, have been named. Naming graphs permits considerable flexibility.

Iizuka et al.[71-74] use the same first step of deriving the graph of a chemical structure in their General Parent Ring System in which block-connected graphs of polycyclic compounds are constructed and systematic notations are derived.

In addition to exploring the feasibility of graph-based nomenclature in which ring systems are numbered by picking a path, which has culminated in the development of nodal nomenclature,[70] CAS, in its search for the "simple integrated system applicable to all types of compounds" that Fletcher[59] also finds desirable, has also been exploring the feasibility of graph-based nomenclature in which component rings of a ring system are numbered in turn. This will be the subject of future papers in this series.

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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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