

In III it is that terminal bond having the lowest degree of unsaturation.

Thus in I, the terminal triple bond has become the dominating factor in establishing the order of carbons in the chain.

When it comes to naming the structures in full, alphabetization of endings must take effect. The IUPAC names of the above are (putting the 1's in)

- I 3-penten-1-yne or pent-3-en-1-yne
- II 1-penten-3-yne or pent-1-en-3-yne
- III 1-buten-3-yne or but-1-en-3-yne

The double bond being senior to the triple bond in IUPAC nomenclature, structure I ought to be named 2-penten-4-yne. Rule A.3-3 has overridden this.

If the logical order of increasing seniority were taken solely as that of increasing unsaturation, single-double-triple, and this were adhered to in all cases of mixed degrees of unsaturation, i.e., if there were a single strict rule for the enumeration of unsaturated structures, the above anomalies would disappear; not only would the naming of these structures be simpler, but computer processing of nomenclature would be less complicated.² But as far as has been ascertained, the IUPAC ruling on the seniority of the double bond has been adopted in other major forms of nomenclature and notation which use a numbering system for chains.³⁻⁶ Only in the author's own development of the Dyson-IUPAC notation, in use from 1965 to 1981, was the strict order suggested incorporated.⁷

Using this suggested order of seniority, IUPAC names for I to III would become

- I 3-penten-1-yne or pent-3-en-1-yne
- II 4-penten-2-yne or pent-4-en-2-yne
- III 3-buten-1-yne or but-3-en-1-yne

It may be argued that for the purposes of nomenclature the single bond does not have to be considered at all, and therefore it does not matter in which order double and triple bonds are placed. An analogy may be that with all organic structures

carbon is considered only after everything else. But in stereoisomerism single bonds have to be considered and are considered last.

CONCLUSION

It is of course not possible to change long-established rules of nomenclature on which many thousands of compounds have been named in the scientific literature. But the purpose of this comment is to point out a seemingly anomalous situation, which it is hoped will not be propagated into any new form of chemical nomenclature or notation which might be suggested for adoption as an alternative, or even eventually a replacement, of present-day IUPAC nomenclature.

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On the Determinant of the Adjacency-Plus-Distance Matrix as the Topological Index for Characterizing Alkanes

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The determinant of the adjacency-plus-distance matrix has been systematically tested for examples that would disprove a supposition that it is a unique topological index (TI) for alkanes. The analysis was carried out for alkane trees with up to 20 sites. The search was fruitful: The first pair of alkane trees with identical TI numbers was already found in the nonane family.

Schultz and co-workers¹ have recently introduced in this journal a novel topological (graph-theoretical) index (TI) for numerical characterization of alkanes. This index was defined as the determinant of the adjacency-plus-distance matrix

$$TI = \det[A + D]$$

where **A** is the adjacency ($N \times N$) matrix and **D** is the distance ($N \times N$) matrix.

The adjacency-plus-distance matrix **A + D** may be directly constructed for the labeled alkane tree. One has simply to input into the distance matrix of an alkane tree the digit 2 in all places where the distance of unity would be otherwise placed.

The authors¹ stated that this index "appears to be useful as a unique molecular topological index for each different alkane". Since the TI is a graph-theoretical descriptor with structural significance, the above statement needs verification. In this paper we will try to answer the important questions "Are the TI numbers unique?", and, if the answer is negative, "What are the smallest alkane trees for which TI is not unique?".

Since we are in the position to generate routinely all alkane trees up to a given number of sites² and have ready a computer program for construction of their distance matrices³ and consequently for their adjacency-plus-distance matrices, we computed the TI numbers for all alkanes with up to 20 atoms

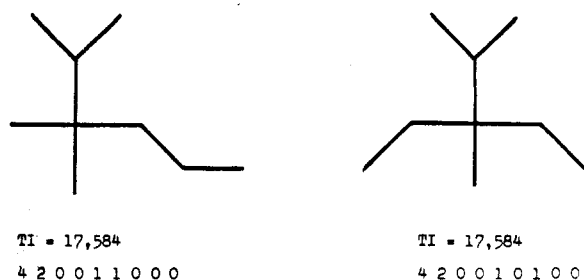


Figure 1. A pair of nonane trees with identical TI's. Beneath each tree its N-tuple code is also given.

(altogether 469 766 alkanes) in our search for nonisomorphic alkane trees with identical TI's. Our target was achieved in the family of alkane trees with nine vertices. A pair of nonanes (2-methyl-2-isopropylpentane and 3-methyl-3-isopropylpentane) possesses the identical value of TI (17 584). These nonane trees, which represent the smallest pair of alkane trees with degenerate TI values, are given in Figure 1. The nonane trees in the figure are also identified by their N-tuple codes² because we used these codes to generate the trees. Thus, the figure contains answers to both questions asked previously. Or, in other words, the TI is not an unique descriptor for characterizing alkanes, and the smallest pair of nonisomorphic alkane trees is diagrammed in Figure 1.

There is another interesting result in the paper by Schultz et al.¹ worth commenting on. They have noticed in their numerical analysis that the distance matrix determinants, $\det|D|$, for each family of isomeric alkane trees have the same values. However, it can be proved⁴ that the determinant of

the distance matrix for all (alkane) trees with the same number of vertices N is given by

$$\det|D| = -(-2)^{(N-2)}(N-1)$$

The above formula also immediately explains the observation of the authors¹ that $\det|D|$ alternates from negative values for all alkane isomers with *even* carbon content to positive values for all isomers of *odd* carbon atom content. The above formula allows quick calculations of $\det|D|$. Thus, one can immediately obtain the value of $\det|D|$ (114 688) for 2,6-dimethyl-5-ethyl-3-isopropyloctane. Schultz et al.¹ obtained a slightly different value (114 687) for this structure. They suspected that their value is not correct because of the value of $\det|D|$ (114 688) for isomeric structures, pentadecane and 2,3-dimethyl-6-ethyl-5-isopropyloctane, and they stated so.

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Online Search Strategies for Semiconductor or Superconductor Materials

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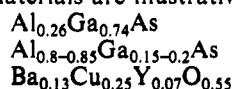
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Recent enhancements introduced by CAS ONLINE and by INSPEC provide powerful new search capabilities for online retrieval of information about nonstoichiometric compositions such as the multitude of fractional atom compounds reported in the literature that deals with, for example, semiconductors or superconductors. In CAS ONLINE, use of the "dot connected atom sequence" permits retrieval of entire families of materials containing specified atoms. In INSPEC, use of the CI field serves a similar function. Illustrative examples of productive search strategies that use these new tools are presented along with a discussion of their limits of applicability.

INTRODUCTION

First-time online searches for semiconductor or superconductor materials can pose unexpected challenges even to experienced practitioners, who are highly skilled in many other areas of chemical searching. These problems arise from a combination of circumstances:

(1) Nonstoichiometric compositions are very prevalent among these families of compounds. The following fractional atom materials are illustrative:



(2) Molecular formula searches and index name searches for these types of compositions in the Registry File of CAS ONLINE or in INSPEC will yield misleadingly small numbers of hits unless special search strategies are utilized that are not

required with other classes of materials.

(3) Both in CAS ONLINE and INSPEC the searcher faces the added complication of working with search strategies that may be applicable only for specific time periods: In both systems the end of 1986 is the dividing line, and distinctly different search procedures are applicable before and after this date. This situation reflects the introduction of helpful new indexing modifications and innovations in these two databases around that time.

(4) Documentation about these problems and applicable search techniques is surprisingly limited. INSPEC issued a series of descriptive pamphlets introducing and explaining the use of chemical indexing (CI) in various online systems such as DIALOG, STN, ORBIT, etc.¹ and also published a superconductor search guide² which, however, contained only a brief reference about chemical indexing as applied to search