the list of atoms with the Morgan algorithm and assigning "parity", even or odd, to each stereocenter.

The class identifiers derived from the topological symmetry algorithm are ideally suited for the assignment of parity to all stereocenters dependent on molecular topology. This perception of stereocenters is not rigorous since there are cases where equivalency may depend upon the chirality of attachments. New class identifiers are needed for a determination of configuration in these cases. For example, consider the diastereomers **17** and **18**. In structure **17** atom 3 is a stereocenter, but not in **18** since the chiralities of the two topologically equivalent attachments are identical. The perception of stereocenters dependent on the configuration of other stereocenters can be achieved by appending the parity property to the class identifier and reimplementing the topological symmetry algorithm.

The algorithm for stereocenter perception may be described as follows: (1) assign class identifiers using the topological symmetry algorithm; (2) use the class identifiers to define the parity of each stereocenter resulting from the molecular topology; (3) append the parity to the class identifier and again partition into classes; (4) reassign the parity of each stereocenter using the new class identifiers; (5) done. It should be noted that chiral structures without stereocenters derived from topological properties are not amenable to this approach. For example, chiral structures **19** and **20** possess no stereocenters that result from molecular topology and require special treatment.

CONCLUSIONS

A simple approach to computer perception of topological symmetry which attempts to mimic that of the chemist has been described. Recognition of the implications of aromaticity is built into the program. The algorithm may be extended to include stereochemical perception.

The algorithm has been used with a large number of examples, and we believe it to be rigorous in the identification of equivalence classes. It is amenable to computer implementation and is efficient and relatively fast in execution. At no time does the algorithm require the examination of atom sets removed by more than one bond from the atom under consideration. This speeds computation since nearest neighbors are explicitly represented by the connection table, whereas further removed atom sets require time for identification.

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(2) The topological representation of molecular structure defines only atom connectivities and element type, and is independent of the three-dimensional nature of the molecule. The term topological symmetry as used in this paper refers only to the symmetry properties of the topological representation. The symmetry properties of the molecular structure differ from its topological symmetry.
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Canonical Numbering and Constitutional Symmetry

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An algorithm is described which assigns numbers to the atoms of a molecular graph in a canonical manner. It is proven that then there is a one-to-one correspondence between the constitution of a molecule and the bond matrix thus numbered. There are no molecules which lead to ambiguities as encountered with other procedures. During the numbering process constitutionally equivalent atoms are recognized. The algorithm is simple enough to be applied directly without any computational support to not-too-complex structures. A computer program based on that algorithm has been implemented and results are given.

I. INTRODUCTION

Coding molecular structures for the manipulation by computers has become of increasing importance.[1] Documentation and information retrieval, computer-assisted synthetic design, and structure–activity correlations are some of the more prominent fields of application. For various purposes a nonunique representation of chemical constitution suffices. But for the storage and retrieval of chemical

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structures a unique description is necessary to avoid multiple storage of the same molecule and to ensure exact matching between query structure and the information to be retrieved.

The extensive work going on in our laboratory in developing computer programs for the solution of chemical problems[2] is based on a mathematical model of constitutional chemistry.[3] A constitutional formula is represented by a BE matrix[3] for which various internal representations are being tested. In our synthetic design program EROS (Elaboration of Reactions for Organic Synthesis), the storage and retrieval of synthetic intermediates are required. As we need access to each in-

dividual atom and bond in a chemical structure, schemes like the Wiswesser Line Notation (WLN)[4] which use codes for groups of atoms were not acceptable to us.

The topology of molecules can be represented by connection tables, lists of bonds, or, equivalently, bond matrices. In the rest of this paper the representation of molecular structures by bond matrices is discussed, but all arguments apply equally to representations by connection tables or indexed lists of bonds. If one represents the topology of a molecule by a bond matrix, there are $n!$ possible numberings of the atoms and up to $n!$ different bond matrices. The task is now to take one of these bond matrices as the canonical one. This is done by numbering the atoms of a molecule in a canonical manner such that a molecule is represented by only one bond matrix.

The constitutional symmetry of a molecular structure should show up in the process of numbering. This is particularly important in synthetic planning or the treatment of chemical reactions by computer, as due consideration of constitutional symmetry avoids the generation of identical precursors or reaction products.

Canonical numbering of the atoms is also necessary for the treatment of the stereochemical features of molecules and reactions.[2c,5]

II. OTHER SCHEMES

There exist already various schemes which attempt to number the atoms of a molecule canonically. The Morgan algorithm[6] used by the Chemical Abstracts Service makes use of the concept of extended connectivity. But as has already been pointed out by Randić,[7] there are some problems with the Morgan algorithm. First, there are cases where the numbering shows oscillatory behavior; i.e., in each iteration different sets of nonequivalent atoms get the same extended connectivity value. Then, with certain structures the extended connectivity values show instability in such a way that although nonequivalent atoms obtain different values their relative ordering changes with each iteration. And finally, for some molecules nonequivalent atoms get the same extended connectivity value in each iteration. Thus, although equivalent atoms get the same extended connectivity value, it cannot always be concluded that atoms with the same extended connectivity value are equivalent.

This problem with the Morgan algorithm has not been resolved by Wipke.[8] Wipke also points out that his algorithm which is based on Morgan's does not always allow the maximum possible differentiation on the basis of connectivity.

Randić[7] uses the eigenvector associated with the largest eigenvalue of the adjacency matrix to number the atoms of a molecular graph. But again there are cases where nonequivalent atoms receive the same index. Further, the eigenvectors had to be looked up in literature;[9] a computer program for the automatic calculation of the eigenvalues of any molecular structure would be rather time-consuming.

III. REQUIREMENTS FOR THE ALGORITHM

Therefore when we embarked on designing a new algorithm for the canonical numbering of the atoms of a molecular graph, we had the following requirements in mind:

1. The algorithm should be unique and a proof for the uniqueness should be given.

2. All constitutionally equivalent atoms should be detected and all constitutionally nonequivalent atoms should receive different indices.

3. The algorithm should use only few rules and these should be simple enough to enable a chemist to number not-too-complex molecules by hand. Further, the algorithm should be easily amenable to programming in any programming language.

4. For different molecules with the same skeleton and differences in the terminal atoms only the skeletal atoms should get the same sequence of indices.

5. The computation time should be small; i.e., the computation time should be short for small molecules and should increase not too much with the number of atoms in a molecule.

6. The storage requirements for the computer program based on that algorithm should be as small as possible to also enable implementation on small machines.

IV. DESCRIPTION OF THE ALGORITHM AND FUNCTION FLOW

In the algorithm, monovalent atoms (hydrogen and nonhydrogen atoms) and nonterminal atoms are treated separately. Thus, as usually, the skeleton built up by the nonterminal atoms is handled first. Terminal atoms are then numbered depending on the numbering of the nonterminal atoms.

Definition: An atom A belongs to the pth neighbor sphere of an atom I if p is the minimum number of bonds between A and I.

Definition: Two atoms are of the same type if they have the same atomic number, the same number of free electrons, and the same number and order of bonds.

Definition: Two bonds are of the same type if the atoms at the end of these bonds and their bond orders are the same.

Definition: Two atoms A and A' are said to be constitutionally equivalent if for each atom X in neighbor sphere p of A there exists an atom X' in p of A' such that X and X' are of the same type. Further, for all bonds starting at X within p and to neighbor sphere $p + 1$ there is a bond of the same type for X' within p and to neighbor sphere $p + 1$ of A', respectively (for $p = 0$ there is A = X, A' = X').

Example 1: Condition i does not suffice for constitutional equivalence since then atoms C_i and C_j would be constitutionally equivalent.
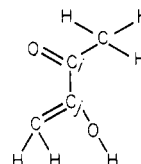
Definition: The number of the outermost occupied neighbor sphere (NOON) of an atom is the minimum number of neighbor spheres necessary to accommodate all atoms of a molecule starting at that atom.

Example 2: NOONs of the atoms of structure 2:
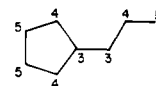
The NOONs of the atoms can be used to exactly define the center of a molecule:

Definition: The center of a molecule is the atoms with the minimum NOON.

Treatment of the Nonterminal Atoms. For each atom the number of the outermost occupied neighbor sphere (NOON) is determined. Atoms which have the same NOON are combined into equivalence classes. These equivalence classes are ordered according to increasing NOONs.

Example 3:

H	D had NOON = 3
G	C, E have 4
A–B–C–D–E–F	F, G, B, J have 5
J	A, H have 6
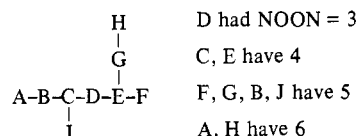
This leads to the following order of equivalence classes: {D} {C,E} {F,G,B,J} {A,H}. Thus, the NOONs have already established a partial ordering.

In the numbering algorithm the atoms within each equivalence class are ordered separately, beginning with the first equivalence class. This leads to a situation that the further an atom lies within a molecule, the lower number it gets. In order to obtain a unique sequence within an equivalence class, for each atom all pairwise combinations with all other atoms of its equivalence class which have not yet been numbered are taken into account. If there are k atoms in an equivalence class, then there are $k(k - 1)/2$ combinations. For each such pair (I,J) the priority of one atom over the other is determined according to the following criteria which are considered in the order given:
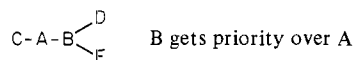
(a) Atomic Number. The atom with the higher atomic number gets priority.

(b) Number of Free Electrons. The atom which has more free electrons gets priority.

The next criteria determine a priority by analyzing the environment of the atoms I,J. The environments of I and J are compared beginning with the α-atoms (first neighbor sphere): All pairs of atoms in the first neighbor sphere of I and J which have the same atomic number and the same bond order to I and J, respectively, are deleted. The remaining atoms in the α-sphere, the bonds between them, and the bonds to the atoms I and J, respectively, are now considered to distinguish between I and J.
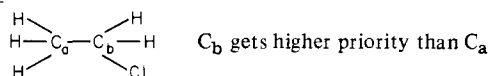
(c) Number of Atoms. The atom which has more (remaining) atoms in the α-sphere gets priority.
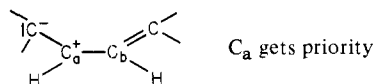
Example 4:

B gets priority over A

(d) Atomic Number of Neighbors. The atom which has an α-atom with higher atomic number than the other gets priority.

Example 5:

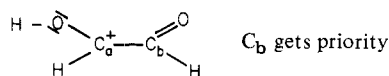C_b gets higher priority than C_a

(e) Free Electrons. The atom which has an α-atom with more free electrons than the other gets priority.

Example 6:

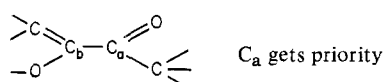
C_a gets priority

(f) Number of Bonds. The atom which has more bonds to the α-sphere gets priority.

Example 7:

C_b gets priority

(g) Bond Priority. The atom with the higher bond order to the heavier α-atom gets priority.
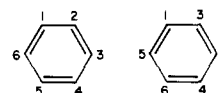
Example 8:

C_a gets priority

If the atoms I and J could not yet be distinguished by taking the α-sphere into account, their environments are the same up to the first sphere. Then the same checks (c – g) are made for the β-atoms (second sphere), etc. If the environments of the two atoms are the same, then no differentiation between

the two atoms can be found, even if all occupied neighbor spheres are taken into account because by definition the atoms are constitutionally equivalent.

Now the task is not yet finished because, if one tries to number constitutionally equivalent atoms arbitrarily, one could end up with different bond matrices for the same molecule.
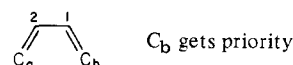
Example 9:

In such cases some additional checks are necessary. This is done by looking for atoms already numbered, whereby one starts with atom 1.

(h) Neighborhood. The atom which lies closer to an atom already numbered gets priority.
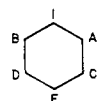
Example 10:

C_b gets priority

(i) Bond Order. The atom which has a higher bond order to an atom already numbered gets priority. This leads to the same bond matrix for different resonance structures for the same charge type, thus solving the problem with benzene (see example 12).

If the atoms cannot be distinguished until now, they are marked as indistinguishable, and all further atoms which can be distinguished are given priority. Then the atoms which were marked indistinguishable are analyzed by rule h to give one of them priority. If no decision is possible, priority is given arbitrarily (see Function Flow below). It will be proved later that at this point arbitrary numbering will lead to a unique bond matrix.

Example 11:

Number 1 has been given arbitrarily. A and B cannot be distinguished and are numbered arbitrarily, say A = 2, B = 3. Now all other atoms are fixed according to rule h: C = 4, D = 5, E = 6.

Example 12:
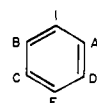
Number 1 has been given arbitrarily. According to rule i B = 2. According to rule h A = 3, C = 4, D = 5, E = 6.

Terminal Atoms. Terminal atoms are numbered according to rule a and h.

Function Flow. As a summary, the function flow of the algorithm will be given.

Given a molecule with arbitrary numbering:

(1) Cut off all terminal atoms.

(2) Determine the minimal number of bonds between all atoms and the number of the outermost occupied neighbor sphere (NOON) for each atom.

(3) Determine the equivalence classes c_k ($k = 1, \ldots, n$). Number the r_k atoms in these equivalence classes c_k arbitrarily from A_k to $E_k = A_k + r_k - 1$ and $A_k = E_{k-1} + 1$.

(4) $k = 0$.

(5) $k = k + 1$.

(6) If $k > n$, then go to (9).

(7) Order the atoms in c_k: *for* I := A_k step 1 *until* E_k *do*; *for* J := I+1 step 1 *until* E_k *do*; check pair (I,J) according to rules a–i. If there are pairs of atoms which cannot be distinguished by rules a through i then:

(7a) In the first run through 4 to 9, make no arbitrary decisions.

(7b) In each following run, make only one arbitrary decision for the first indistinguishable pair of atoms.

(8) Go to (5).

(9) If there are remaining pairs of indistinguishable atoms, go to (4).

(10) Number the terminal atoms according to rules a and h.

(11) End.

Note: The algorithm is always finite: In each run through (4) to (9) at least one atom of an indistinguishable pair (I,J) is given priority.

V. PROOF OF THE UNIQUENESS OF THE NUMBERING

It has to be shown: For any starting numbering of a molecule M there exists only one unique bond matrix of M which represents the numbering after running through the algorithm.

Proof: (indirect)

Assumption: For a molecule M there exist two different starting numberings, for which the algorithm generates two different "unique" bond matrices U and U' with $U \neq U'$.

From this assumption follows that there is a permutation matrix P with

$$U = PU'P^T$$

The permutation which is represented by P may be (i,j,k,l,m) (cyclic notation). As each permutation, (i,j,k,l,m) can be written as a sequence of transpositions, we have:

$$(i,j,k,l,m) = (i,j)(j,k)(k,l)(l,m)(m,i)$$

Then to disprove the assumption, it has to be shown, that either the algorithm is able to give one atom of each pair (I,J) priority or, if this is not possible, that the two possible generated numberings (depending on the starting numberings) lead always to the same bond matrix.

Since the algorithm checks all bonds between all neighbor spheres and within them and also all atoms in all neighbor spheres of any two atoms I,J, it can always distinguish between two constitutionally *nonequivalent* atoms and thereby determine priority. Further constitutionally *equivalent* atoms which are covered by rules h and i can also be distinguished. Thus it suffices to consider only those pairs of constitutionally *equivalent* atoms which cannot be assigned by rules h and i.

It can be disproved by induction that then there exists a case where an arbitrary numbering of atoms I,J which cannot be distinguished by the algorithm leads to two different BE matrices.

(i) No atom has yet been assigned, i.e., I = 1, J = 2 or I = 2, J = 1. Without limiting the validity of the proof, it can be assumed that no atom has a higher priority than I or J because otherwise one would not yet have to assign I or J. The two possible assignments lead to the same bond matrix because then the matrix has at most one entry: the bond I–J, if there is one at all.

(ii) Atoms have already been assigned. Without limiting the validity of the proof it can be assumed that all atoms which lie closer to the center than I or J have already been assigned because otherwise one would not yet have to assign I or J. (It is possible that also atoms which lie farther away from the center than I or J have already been assigned as will be the case with polycyclic compounds.) Let us assume that all direct neighbors of I and J, which can be given priority without making a decision for I and J, have already been assigned. If then I and J cannot be differentiated, they must have in common all assigned direct neighbors because otherwise they could be given priority through rule h. Then, if I and J have all assigned direct neighbors in common, the two choices for assigning I and J must lead to two identical bond matrices. If I and J have also direct neighbors which have not yet been

assigned, their assignment instead can also not lead to ambiguities as their priority is dependent on the assignment of I and J. (Otherwise they would have already been assigned.)

The two choices for assigning I and J lead in each case to two identical bond matrices. This disproves the original assumption, thus showing that the algorithm generates a numbering which leads to a unique bond matrix.

VI. COMPUTATIONAL RESULTS

The program is written in PL/1 and run on an IBM 360/91. The computation time necessary for numbering a molecule is rather independent of the starting numbering. However, if only the terminal atoms have to be renumbered, the computation time is only a fraction of the time necessary for numbering the whole molecule.

Factors which increase the computation time are the following.

(i) Molecules with large ring systems (e.g., coronene): The determination of the neighbor spheres of the atoms in such molecules needs more computation time, because there are many paths to be considered in going from one atom to another.

(ii) Molecules with many constitutionally equivalent atoms (molecules with high symmetry): All neighbor spheres of constitutionally equivalent atoms have to be checked as no discrimination is found.

Storage Requirements. Let nb be the number of bonds, na the number of atoms, and nas the number of atoms with more than one bond. In the program, storage space is allocated dynamically. The maximum storage required for matrices and vectors (depending on the size of the equivalence classes) is:

$$2(6nb + (10 + nas)na + (2 + nas)nas + \sim 50) \text{ bytes}$$

e.g., for a molecule with 30 atoms, storage space of about 3.2K bytes is required.

Test Runs. The computation times are averages obtained on several runs. The times include renumbering and reordering of the bond matrix: benzene, 0.26 s; naphthalene, 0.41 s; anthracene, 0.95 s; coronene, 2.9 s.

The ratio of these computation times is 1 : 1.58 : 3.65 : 11.15. The ratio of the number of atoms with more than one bond is 1 : 1.7 : 2.34 : 4. From that it can be deduced that the computation time increases with less than the square of the number of atoms with more than one bond.

Molecules without rings need less computation time: methane, < 0.01 s; pentane, 0.17 s; ethyl acetoacetate, 0.19 s.

VII. CONCLUSIONS

An algorithm for the canonical indexing of the atoms of molecules has been developed. Although the discussion centered around molecular graphs, this algorithm can be quite generally applied to labeling weighted graphs. All the requirements we wanted to impose on the algorithm on the outset of this work (see section III) could be met.

As was proven, this procedure generates for each molecular structure a numbering of the atoms which leads to one unique bond matrix as a representation of this molecule, thereby solving problems other systems[6-8] could not handle. In many cases the indexing is the same as the one obtained by the widely used Morgan algorithm,[6] but the pitfalls[7,8] of this algorithm have been avoided.

In the process of numbering the atoms of a molecule, the algorithm detects all constitutionally equivalent atoms, thereby giving access to overall and local symmetry of the molecule. Further, an exact definition of the center (centers) of a molecule or a graph could be given. This has implications also

for generating a two- or three-dimensional picture of the molecule from the list of bonds or from the bond matrix as there a knowledge of the center of the molecule is quite helpful. Another advantage is that changes in the substitutional patterns of the monovalent atoms do not affect the indexing of the skeleton.

The rules employed in the algorithm are few and simple enough to allow a chemist to number not-too-complex structures easily by hand. Further, a computer program has been implemented on the basis of this algorithm which automatically handles any structure fast and with a small amount of storage space.

ACKNOWLEDGMENT

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————————NEWS AND NOTES————————

NEWS ITEMS

Parent Compound Handbook

A new handbook containing structure diagrams, names, and other identifying information for more than 40,000 cyclic, acyclic, and cage structures whose names provide the parent index headings under which related substances are grouped in the *Chemical Abstracts* indexes now is available from Chemical Abstracts Service. The "Parent Compound Handbook", which replaces and brings up to date and expands the coverage of the 1960 edition of the "Ring Index" and its supplements, includes information compiled by CAS over more than half a century.

The listing for each compound in the handbook provides a structure diagram showing preferred orientation and nomenclature locants, the name under which the compound is indexed in *Chemical Abstracts*, its CAS Registry Number and molecular formula, and, in most instances, its Wiswesser Line Notation and a ring analysis of the type used in the CA Index of Ring Systems. This information is contained in a two-volume Parent Compound File, one volume of which is issued in a loose-leaf binder. Six indexes in a separately bound Index of Parent Compounds provide access to the content of the Parent Compound File via name, Registry Number, ring analysis, ring substructure, molecular formula, and Wiswesser Line Notation.

CAS will keep the "Parent Compound Handbook" up to date by issuing supplementary pages for the Parent Compound File on new parent structures encountered in the CAS Chemical Registry System and cumulative indexes to the supplementary material. Supplements will be issued every other month beginning in June 1977. The handbook's $200 price includes updating service through 1978. A revised Index of Parent Compounds incorporating all supplementary material will be published every two years.

For additional information on the "Parent Compound Handbook", contact the Marketing Department, Chemical Abstracts Service, Box 3012, Columbus, Ohio 43210.

CAS Names Advisors

Appointment of five new members and reappointment of one member to the advisory board of Chemical Abstracts Service have been announced by CAS Director Dale B. Baker.

New members of the board, named for three-year terms, are Mr. William S. Budington, Executive Director and Librarian, The John Crerar Library; Mrs. Margaret H. Graham, Exxon Research and Engineering Co.; Dr. Berwyn E. Jones, Professor of Chemistry, Upper Iowa University; Dr. William T. Lippincott, Editor, *Journal of Chemical Education*, and Professor of Chemistry, University of Arizona; and Dr. William E. McGonigal, Director, Experimental Station Laboratory, Biochemicals Department, E. I. du Pont de Nemours & Co.

Dr. Willis H. Ware, Corporate Research Staff, Rand Corporation, has been reappointed to the board for a second term.

Other current board members are: Mr. A. H. Epstein, Stanford University; Dr. Helmut Gruenewald, Gesellschaft Deutscher Chemiker; Dr. Allan S. Hay, General Electric Co.; Professor Sir Ewart Jones, Dyson Perrins Laboratory, Oxford University; Dr. Anthony K. Kent, United Kingdom Chemical Information Service; Mr. Frederick G. Kilgour, Ohio College Library Center; Mr. Donald W. King, King Research, Inc.; Dr. Michael E. Lesk, Bell Telephone Laboratories; Dr. Cyrus Levinthal, Columbia University; Mrs. Cynthia H. O'Donohue, Philip Morris Research Center; Mr. David E. Sparks, Notre Dame University; Mr. Kermith H. Speierman, Department of Defense; and Mr. Peter F. Urbach, National Technical Information Service.