Personal Microcomputer Based System of Chemical Information with Topological Structure Data Elaboration

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A program of chemical information handling, ARIUSA, running on PC-AT microcomputers, with a structural data elaboration step is described. Thus after a structure is input, the system elaborates it in order to get further information such as molecular formula, molecular weight, and the Wiener, Randic, and Balaban topological indices. In the alphanumeric retrieval of different attributes the numerical information can be searched as a fixed value or as a particular range. The program can retrieve molecular structures for which the molecule of interest is identical, a substructure, or a superstructure, and also all of these with variable atoms and bonds, which makes possible a similar structure search. The retrieval can be further refined by using the AND and NOT functions. In addition, it allows one to work with a summary of the references where graphic correlations are included. This system has been specially designed as a tool in organic synthesis and in the search of structure–property and structure–activity relationships.

INTRODUCTION

One of the oldest methods of communication of chemical knowledge is the alphanumeric and graphic representation of structures and correlations. With the appearance of microcomputers of growing capacity, it is now desirable to manage, in an automatic form, all of the growing information in a way similar to the manual writing used for handling a small number of references, profiting from the advantages offered by these machines. However, the facilities offered by microcomputers in this field still have to be worked out because they normally help only with the alphanumeric information within a database.[1,2] On the other hand, the importance of a number of correlations between the molecular structure and some physical, chemical, or biological molecular properties has created the necessity of translation of the structure of a molecule into a numerical descriptor.[3] In effect, these numerical descriptors, which take into account the shape and the volume of the molecule, are known as topological indices. These indices take into consideration how many atoms there are in the molecule, how many atoms are connected to each one within the molecule, and whether the atoms are connected to form a single straight chain, a straight chain with branches, or rings. Even though these topological indices have been widely used for predicting physical, chemical, and biological properties,[3,5-11] they do not take into consideration the stereochemistry of the molecules. These points have been highlighted in this paper, and for the first time they have been implemented in a microcomputer information system.

We recently developed a microcomputer system called ARIUSA, running under CPM with a Z-80 CPU,[4] and also its IBM-PC version, written in Pascal, for storage and retrieval of chemical information. In this paper we describe further development of that program, now running under DOS with an 80286 and also an 8088 CPU. This improved system allows one to handle not only the normal alphanumeric input information (title, authors, journal, location, keywords, subjects) but also a summary of the reference, the name of the molecules, and the graphic molecular structures with their stereochemistry. Also, it further elaborates the stored molecular structure data in order to get extra information about the molecule such as (a) molecular formula, (b) molecular weight, and (c) topological indices.

Retrieval of information can be done by using any of the attributes as search restrictions (conditions imposed to the search). Because of the predictive value topological indices have, the proper handling of these quantities could have considerable importance in the establishment of new structure–property relationships or as a tool in molecular design. Additionally, the search step includes retrieval of references containing molecular structures with a particular maximum or minimum number of different atoms and variable bonds. It also incorporates a refinement of retrieval with the AND and NOT functions.

GENERAL DESCRIPTION OF THE SYSTEM

The system ARIUSA has five steps: INPUT, STRUCTURAL DATA ELABORATION, RETRIEVAL, REVIEW AND MODIFICATIONS, and OUTPUT. Each of these steps has several menus, thus making ARIUSA a menu-driven system. All of the menus are made in such a way that answering them and following the process is a very straightforward procedure.

(1) INPUT Step. The input of information can be made either alphanumerically or graphically.

(a) Alphanumeric: ARIUSA allows for the introduction of a part or all of the information that is normally handled in chemical references including keywords, journals, authors, and so on. For the input of the information the user has to fill in the chart shown in Figure 1. It can also store a summary of the publication, and this is done interactively. In the same way, the name of the molecules of the publication can be stored as a separate attribute.

(b) Graphic: Graphic input works with molecular structures where the stereochemistry is one of the attributes. It considers implicit and explicit atoms and the representation of some specific common groups such as acetate, *o*-toluenesulfonate, and phenyl as a single superatom. The input is done interactively with the help of five menus that allow the user to select the type and position of the atoms, the type and stereochemistry of the bonds, the charge of the atoms, the closure of a ring, or the addition of a substituent. This is done simply making use of the numerical pads of the microcomputer keyboard. A graphic tablet may also be used.

(2) STRUCTURAL DATA ELABORATION Step. After the molecular structure has been introduced, ARIUSA allows for the obtention of information that is not normally offered by the reference itself. This means the program can get some extra attributes from the structure such as molecular formula, molecular weight, and topological indices. Because of their simplicity and importance, the Wiener index, the Randic index, and the Balaban index have been used in this work.

The Wiener index is based on the graph-theoretical notion of distance: the distance between any two vertexes (carbon or heteroatoms) is equal to the number of edges (bonds) one would traverse in taking the shortest possible route through the molecule's graph (skeleton) from one of the vertexes to

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```
Title     :

Authors   :

Journal   :

Location  :

          KEYWORDS                    SUBJECTS
     1.-                         1.-
     2.-                         2.-
     3.-                         3.-
     4.-                         4.-
     5.-                         5.-
     6.-

          AFTER THE INPUT IS FINISHED PRESS PGDN
```

Figure 1. Alphanumeric information input chart.

```
Title:.............................

Authors:...........................

Journal:...........................

Location:..........................

Keyword:..............

Subject:..............          Molecular  Formula: .........

Molecule name:..................

          ..... <= Mol. Weight <= .....

          ..... <=  Degree     <= .....

          ..... <=  Distance   <= .....

          ..... <=  Centric    <= .....
```

Figure 2. Alphanumeric retrieval search chart.

the other. For example, in *n*-pentane the graph-theoretical distance between carbon 1 and carbon 5 is four. The Wiener index of a molecule is equal to the sum of the graph-theoretical distances between all pairs of atoms in the molecule.[5]

The Randic index considers that each vertex has a "degree", the number of other vertexes it is linked to. Similarly, each edge has a "value", the product of the reciprocals of the square roots of the degrees of the vertexes it joins. The Randic index of a molecule is equal to the sum of the values of all of the molecule's edges.[6]

The Balaban index considers principally the degree of branching in a molecule. All vertexes that are linked to just one other vertex (e.g., a primary carbon atom) are counted and "pruned" from the molecule's graph. The number of vertexes pruned at each step is squared and added to a running total. The process is repeated until every vertex has been counted. The Balaban index is the final total.[7]

All of these attributes generated by the system fill out the alphanumeric information chart of each reference.

(3) RETRIEVAL Step. The retrieval of information can be done by using alphanumeric or graphic restrictions or both of them.

(a) Alphanumeric: ARIUSA is able to retrieve all of the references under one or all of the alphanumeric attributes (or a part of them). It can also retrieve information under a range of topological indices values generated in the data elaboration step. The range value can be limited at one or both extremes as is shown in Figure 2.

(b) Graphic: This is used to retrieve information related to molecular structure. The target molecule must be drawn first; the procedure is similar to the graphic input of information. Then it is possible to start the search by looking for an identical structure or a similar structure having the same number of atoms and bonds, with the alternative of considering variations in the type of the atoms and/or bonds. Also, it is possible to search for molecules having a larger number of atoms (substructure search) or a smaller number of atoms (superstructure search) than the target molecule. The number of extra or fewer atoms and also the alternative of different

```
                                   time                 date
title     :
authors   :
journal   :
location  :                        summary  :
keyword1  :                        subject1 :
keyword2  :                        subject2 :
keyword3  :                        subject3 :
keyword4  :                        subject4 :
keyword5  :                        subject5 :
keyword6  :                        MWeight1 :
MWeight2:.....  MWeight3:.....  MWeight4:.....  MWeight5:....
          name              formula  degree  distance  centric
mol1 : ........              ...      ...     ...       ...
mol2 : ........              ...      ...     ...       ...
mol3 : ........              ...      ...     ...       ...
mol4 : ........              ...      ...     ...       ...
mol5 : ........              ...      ...     ...       ...
```

Figure 3. Review and modifications chart.

atoms and/or bond types can be selected at will on the interactive menus. In addition, it is possible to search at the same time under both substructure and superstructure options.

(c) Graphic and Alphanumeric: This is used to put specifications or restrictions on the search combining both previous steps, thus making the process more selective. Once the references have been found according to the restrictions introduced during the search, ARIUSA allows for a further search on them in order to get a more refined retrieval. This is done by using the functions AND and NOT. These functions allow for the selection of attributes that match or do not match some new imposed restrictions to the previously found references. After the information is finally selected, it is ready for output.

(4) REVIEW AND MODIFICATIONS Step. The user can review the alphanumeric and graphic information of the references found with or without any restriction, which are shown one by one as Figure 3 indicates. This is done through the use of previously defined commands in the forward or backward direction. Also, it is possible to get at once the first of the found references or the last of them. In this step it is possible to modify the information on the screen or to mark a reference in order to be printed or deleted afterward. If a molecule is added, deleted, or modified, all of the remaining associated information is automatically updated.

(5) OUTPUT OF THE INFORMATION Step. There are two output options that can be chosen from a menu: to print all of the found references or to print a selected number of them. In addition, only the fields that have been occupied during the input step are shown on printing. Also, if the summary is included in the reference, it can optionally be printed.

The graphic restrictions used during the retrieval are shown in the first page of the printed alphanumeric information corresponding to the found references. Graphic representation for each of these references is not done. This is in acccord with the actual availability of peripherals, the time of printing, the resolution of peripherals, and their usefulness.

COMPUTATIONAL DESCRIPTION

The computational organization of the whole ARIUSA system is described below (see Figure 4). The input of the alphanumeric information is handled by the program INPUT, written in dBase, which creates records in the ARIUSA database with the characteristics indicated in Table I.

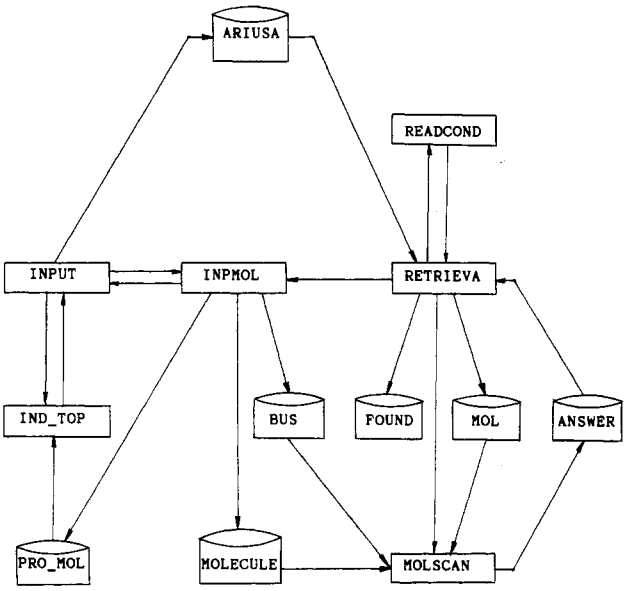

Figure 4. Diagram of ARIUSA architecture.

Table I. Structure of ARIUSA Database Records

field	field name	type	length
1	TITLE	character	254
2	AUTHORS	character	80
3	JOURNAL	character	80
4	LOCATION	character	80
5	KEYWORD1	character	20
10	KEYWORD6	character	20
11	SUBJECT1	character	20
15	SUBJECT5	character	20
16	MOLECULE1	character	30
17	MOLECULE2	character	30
18	MOLECULE3	character	30
19	MOLECULE4	character	30
20	MOLECULE5	character	30
21	NR_MOL1	numeric	6
22	NR_MOL2	numeric	6
23	NR_MOL3	numeric	6
24	NR_MOL4	numeric	6
25	NR_MOL5	numeric	6
26	DEGREE1	numeric	6
30	DEGREE5	numeric	6
31	DISTANCE1	numeric	8
35	DISTANCE5	numeric	8
36	CENTRIC1	numeric	3
40	CENTRIC5	numeric	3
41	FORMULA1	character	20
45	FORMULA5	character	20
46	MWEIGHT1	numeric	5
47	MWEIGHT2	numeric	5
50	MWEIGHT5	numeric	5
51	SUMMARY	memo	10

The input of the graphic information is handled by the program INPMOL, written in Pascal. This program is called by INPUT with an A code (Add). The codified molecule is stored by INPMOL in some available space of the relative archive MOLECULE. This archive has the characteristics shown in Table II. INPMOL returns to INPUT a number with the physical location of the molecule, and INPUT returns that information to the ARIUSA database. Finally, the molecule's physical location number is located in one of the database fields named NR_MOLi with $1 \leq i \leq 5$. All of the molecules of a reference are input one by one via this procedure. In Figure 5 the relationships that exist between the data structures of the alphanumeric and the graphic archives of Tables I and II are shown.

Once the molecular structure is stored, the system starts the data elaboration step for the attributes molecular formula,

Table II. Characteristics of the MOLECULE Relative Archive

```
CONSTANTS
  MAX_AT = 30;
  MAX_BN = 32;
  X_MAX = 639;
  Y_MAX = 195;
  NATCHT = 10;
TYPE
  R_ATOMS = 0..MAX_AT;
  R_BONDS = 0..MAX_BN;
  R_COOR_X = 1..X_MAX;
  R_COOR_Y = 1..Y_MAX;
  R_CHARGE = 0..4;
  TYPE_ATOM = 1..255;
  T_BOND = 0..255;
  T_COOR_X = ARRAY [1..MAX_AT] OF R_COOR_X;
  T_COOR_Y = ARRAY [1..MAX_AT] OF R_COOR_Y;
  T_TYPE_A = ARRAY [1..MAX_AT] OF TYPE_ATOM;
  T_TYPE_E = ARRAY [1..MAX_BN] OF T_BOND;
  T_CHARGE = ARRAY [1..MAX_AT] OF R_CHARGE;
  T_ATOM = ARRAY [1..MAX_BN] OF R_ATOMS;
  MOL_CODI = RECORD
    ATALPHA : ARRAY[1..MAX_AT,0..NATCHT] OF
    R_ATOMS;
    ORDER : ARRAY[1..MAX_AT,1..MAX_AT] OF
    T_BOND;
    ATTYPE : T_TYPE_A;
    CHARGE : T_CHARGE;
    BNTYPE : T_TYPE_E;
    COOR_X : T_COOR_X;
    COOR_Y : T_COOR_Y;
    NR_AT : R_ATOMS;
    NR_EST : INTEGER;
    END;
    WORD = 0..255;
  T-REG = RECORD
      MOL_COD : MOL_CODI;
      NEXT : INTEGER
    END;
  MOLECULE = FILE OF T_REG;
```

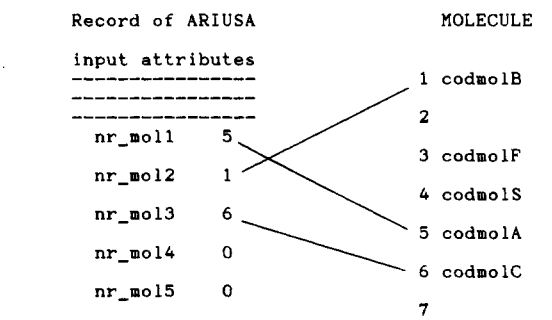

Figure 5. Relationships between the archives ARIUSA and MOLECULE.

molecular weight, and the three topological indices. For this purpose, INPMOL calculates the molecular formula and the molecular weight of each of the stored molecules. It also generates the archive PRO_MOL, where the codified molecule data for each of the molecules of the reference are stored with a format ready to be read by the program IND_TOP, written in Prolog, which calculates the topological indices. All of this information is returned to INPUT to be stored in the alphanumeric information ARIUSA database.

The retrieval process is controlled by the program RETRIEVA, written in dBase. RETRIEVA calls the program READCOND, written in Pascal, for reading the alphanumeric restrictions imposed by the user to the search. RETRIEVA generates a temporary archive called FOUND, where the number of the found references that matches the alphanumeric restrictions is stored.

When molecular restrictions are imposed to the search, this is done only over the temporary archive FOUND and a new archive called MOL, having the number of references containing

```
..... PUBLICATIONS WERE FOUND

1.- Do you want to see them?

2.- Do you want to put more restrictions on them?

3.- Do you want to begin a new search?

4.- Do  you want  to print  all of them?

5.- Do you want to print the publications with marks?

6.- Do you want to erase the publications with marks?

7.- Do you want to finish the search?

8.- Do you want to quit?
```

Figure 6. Menu of the final found references.

molecules and their respective physical location number on MOLECULE, is generated by RETRIEVA. RETRIEVA also calls the program INPMOL for reading with a D code (Drawing) the target molecule. This program generates an archive, called BUS, with the codified data of the target molecule.

After the above steps, MOLSCAN, written in Pascal, is called by RETRIEVA for doing the molecular search. The number of the molecules to be searched is taken from MOL. With these numbers MOLSCAN takes from MOLECULE the corresponding codified structures, which are compared with the codified target structure taken from BUS. The search algorithms used[4] are a combination of a quick preliminary scan followed by a more accurate atom by atom search starting from the more chemically discriminant atom. Finally, an archive with the references having the correct alphanumeric and graphic restrictions, called ANSWER, is generated by MOLSCAN. The menu with the results of the retrieval is shown in Figure 6 together with several options to proceed with.

As said above, ARIUSA is written in Pascal, in dBase III, and in Turbo Prolog and runs on an IBM-PC microcomputer with 512-KB RAM. The system works with two disk drives or with a hard disk running under DOS version 3.00, with a graphic display of medium resolution of 640 × 200/350 pixels. The microcomputer works with any printer (Epson MX-100 with graphic capabilities in our case). Each diskette of 346 KB can store about 200 references having one drawn molecule.

A hard disk is recommended for better performance and storage capacity. An average publication with two molecules and a summary of 512 characters occupies 2950 bytes; that means about 13 600 publications can be stored in a 40-MB hard disk.

DISCUSSION AND CONCLUSIONS

This system has a versatile mode of handling information. The input can be done both in alphanumeric mode, including a summary, and in graphic mode. It has an automatic data elaboration step based on the graphic input structures. The retrieval is highly refined according to the user restrictions through menus that use the AND and NOT functions.

The system permits us to modify the graphic or alphanumeric information anytime during the input or retrieval steps. This allows one to store the full information or partial information from a *Current Contents* issue, for instance. After checking it into a primary source, it is possible to complete it or to delete the partial information.

With the possibility of working with text storage it is possible to keep an extended summary of the information. In this way we can store the most relevant information according to our needs, sticking to the old but effective manual method used for a small number of references.

Within the graphic capabilities of the system, the stereochemical attributes seem to have interest when a particular publication has associated chiral compounds, as is the case in asymmetric synthesis or in the description of bioactive compounds such as pheromones. Using its graphic capabilities, ARIUSA can retrieve information under (a) identical structures, (b) similar structures (different atoms and bonds), (c) identical and similar substructures, (d) identical and similar superstructures, and (e) simultaneous identical or similar superstructures and substructures. For using substructures or superstructures the user has to define the extra or fewer number of atoms, and this is done through a menu offered by the program.

The combination of these structural strategies of searching with the use of convenient alphanumeric restrictions will allow the user to have a different perspective of the stored information. In this way ARIUSA will help to analyze in a creative way the information found and to make a contribution to areas such as molecular design.

The data elaboration step based on the drawn molecular structures complements the alphanumeric information introduced at the input step. Thus the molecular formula and the molecular weight are two extra parameters usually needed during an exhaustive chemical information search. The time used by ARIUSA to calculate these parameters and the topological indices discussed below is between 1 and 3 s.

The topological indices included in the data elaboration step of ARIUSA allow for the prediction, confrontation, or at least an estimation of some molecular properties on the basis of correlations previously established.[3] These indices are introduced here just as an example of how molecular structures can be characterized with a unique numerical descriptor that then helps in finding correlations between the structure and some properties. As the mathematical expressions that describe the three mentioned indices are known, calculating them for any molecule is straightforward, and that is what ARIUSA does each time a molecule is stored. According to user convenience, another index could be easily introduced in ARIUSA because of the modular programming of the system. So each user could calculate a particular index for a molecule immediately after the structure of the molecule has been stored.

The Wiener index, for instance, correlates very well for a number of alkanes, alkenes, and alkynes for several physical properties such as melting point, boiling point, viscosity, density, surface tension, and heat of vaporization.[5,8-11] On the basis of a known correlation of the Wiener index with a particular property for a group of compounds, it is possible then, by knowing the value of the index, to find the property for any molecule of the group. Also, ARIUSA can help to solve the inverse problem—to find molecules with a particular property. For that, ARIUSA makes a retrieval under the index or the range of values of topological indices which correlates better with the desired property.

Important to the method of using topological indexes is to find the index that correlates best with the property being studied. In that sense it is sometimes necessary to combine topological indices in order to get a good correlation with a particular property. All of that can create a specialized topological index. From this point of view ARIUSA is a useful tool for scientists already working with topological indices and also for those who have not worked with these concepts yet. Now they may find out in an easy way if there is any correlation between any particular property of interest, for a group of compounds, and the implemented topological indices.

The speed of processing of the information (retrieval) depends on the unit and the CPU used. Table III gives a comparison for a database of 250 references searched under alphanumeric restrictions. Search time increases by a factor of 1.3–2.0 when the search is done with molecular restrictions. ARIUSA runs best when it works, under DOS, with a virtual disk. The storage capacity certainly depends on the unit used. With the increasing capacity of microcomputers it will be

Table III. Response Time in Function of the Hardware for an Alphanumeric Retrieval over 250 References

unit	processor	response time
two disk drives	8088 (4.7 MHz)	3 min
two disk drives	80286 (10 MHz)	1.5 min
one hard disk	80286 (10 MHz)	10 s
one virtual disk	80286 (10 MHz)	4 s

possible for this type of personalized system to acquire more diffusion among users because it solves the ordinary problems generated with the handling of increasing numbers of references.

On one side, ARIUSA can take advantage of molecular structures with a known stereochemistry; on the other side, it can take advantage of the graph theory where the stereochemistry is not considered at all but where it is possible to retrieve some new useful information. These enhancements make of ARIUSA a different personal system of chemical information, useful for a wide range of users.

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REFERENCES AND NOTES

(1) Ash, J. E.; Chubb, P. A.; Ward, S. E.; Welford, S. M.; Willet, P. *Communication, Storage and Retrieval of Chemical Information*; Ellis Horwood: Chichester, England, 1985.
(2) Smith, S. F.; Jorgensen, W. L.; Fuchs, P. L. "PULSAR: A Personalized Microcomputer-Based System for Keyword Search and Retrieval of Literature Information". *J. Chem. Inf. Comput. Sci.* **1981**, *21*, 209-213.
(3) Bonchev, D. *Information Theoretic Indices for Characterization of Chemical Structures*; Research Studies: New York, 1983.
(4) Contreras, M. L.; Deliz, M.; Galaz, A.; Rozas, R.; Sepulveda, N. "A Microcomputer-Based System for Chemical Information and Molecular Structure Search". *J. Chem. Inf. Comput. Sci.* **1986**, *26*, 105-108.
(5) Wiener, H. "Structural Determination of Paraffin Boiling Points". *J. Am. Chem. Soc.* **1947**, *69*, 17-20.
(6) Randic, M. "On Characterization of Molecular Branching". *J. Am. Chem. Soc.* **1975**, *97*, 6609-6615.
(7) Balaban, A. T.; Motoc, I. "Chemical Graphs. XXXVI. Correlations between Octane Number and Topological Indices of Alkanes". *MATCH* **1979**, *5*, 197-218.
(8) Rouvray, D. H. "Predicting Chemistry from Topology". *Sci. Am.* **1986**, *255*(3), 36-43.
(9) Platt, J. R. "Prediction of Isomeric Differences in Paraffin Properties". *J. Phys. Chem.* **1952**, *56*, 328-336.
(10) Rouvray, D. H. "The Values of Topological Indices in Chemistry". *MATCH* **1975**, *1*, 125-134.
(11) Rouvray, D. H.; Crawford, B. C. "The Dependence of Physicochemical Properties on Topological Factors". *S. Afr. J. Sci.* **1976**, *72*, 47-61.

Computer Simulation of Deuterium NMR Line Shapes

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The results of a computer program written to study rotational dynamics by following the reorientation of a carbon-deuterium (C-D) bond vector in a deuteriated molecule are described. Three-dimensional plots are constructed to show how deuterium nuclear magnetic resonance splittings vary as a function of two rotational parameters. It is suggested that these diagrams provide insight into the rotational motions of the molecule.

INTRODUCTION

One of our principal research objectives is to investigate polymer dynamics by using, among other techniques, deuterium nuclear magnetic resonance (DNMR) as a probe. In contrast to the proton, deuterium has a nonzero quadrupole moment (2.73×10^{-3} barns), low abundance (0.015%), and a small magnetogyric ratio (15.3% of the proton value). Consequently, DNMR spectra are remarkably simple compared to conventional proton NMR spectra. The rationale for this is as follows: The nonzero quadrupole moment means that experimental results (relaxation times and line shapes) for deuterium can be directly related to the reorientation of C-D or O-D bond vectors. This is an intra- and not an intermolecular effect. Since C-D bonds often have axially symmetric electric field gradients, the interpretation of line shapes and relaxation times are simplified. The low abundance allows specific labeling with deuterium in any position, and it assures that the resulting DNMR spectrum only contains a contribution from deuterium in that position. The background signal from unlabeled positions is relatively negligible. This is an important advantage in concentrated solutions and bulk polymers, for example, where conventional proton NMR and ^{13}C NMR resonances may strongly overlap. Also, if only one position is labeled per monomer unit, the label does not significantly perturb the translational and rotational motion of the molecule. Finally, the relatively small magnetogyric ratio of the deuterium results in a comparatively small dipolar coupling effect. As a result of this the complicated spin-diffusion effects often seen in protonated polymers are not active in deuterium NMR.

There are many examples in the literature of how DNMR spectra are used to elucidate motions in small molecules and polymers. Jelinski et al.[1-3] have probed the anisotropic reorientation of water in an epoxy system as well as studied ring flips in collagen. Jelinski et al.[4] have also used DNMR to test the validity of "three-bond" motions in polymers. Opella et al.[5,6] have investigated ring flips and other motions in phenylalanine. Blum et al.[7] have shown how DNMR relaxation times can probe molecular motion in very concentrated polymer solutions and gels. They have also used DNMR to correlate polymer backbone dynamics with translational motion of the solvent.[8] Spiess[9,10] has described the versatility of DNMR for studying a wide variety of problems over a very wide time scale and DNMR of liquid-crystalline polymers has also been reviewed.[11]

Thus far it has proved impossible to determine molecular dynamics of systems from first principles and a combination of NMR line shapes and relaxation times. Consequently,

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