tinic Pharmacophore. *J. Med. Chem.* **1986**, *29*, 899-906.
(8) Takahashi, Y.; Maeda, T. S.; Sasaki, S. Automated Recognition of Common Geometrical Patterns Among a Variety of Three-Dimensional Molecular Structures. *Anal. Chim. Acta* **1987**, *200* (1), 363-377.
(9) Ghose, A. K.; Crippen, G. M.; Revankar, G. R.; McKernan, P. A.; Smee, D. F.; Robins, R. K. Analysis of the in Vitro Antiviral Activity of Certain Ribonucleosides against Parainfluenza Virus Using a Novel Computer-Aided Receptor Modeling Procedure. *J. Med. Chem.* **1989**, *32*, 746-756.
(10) Takahashi, Y.; Akagi, T.; Sasaki, S. Three-dimensional pharmacophoric pattern search using COMPASS: Nootropic Agents. *Tetrahedron Comput. Methodol.* **1990**, *3*, 27-35.
(11) Austel, V.; Muller, P.; Reiffen, M. Systematic Consideration of Conformational Properties in Series Design. In *QSAR in Drug Design and Toxicology*; Hadzi, D., Jerman-Blazic, B., Eds.; Elsevier Science Publishers B.V.: Amsterdam, 1987; pp 85-89.
(12) Jakes, S. E.; Willett, P. Pharmacophoric Pattern Matching in Files of 3-D Chemical Structures: Selection of Interatomic Distance Screens. *J. Mol. Graphics* **1986**, *4*, 12-20.
(13) Jakes, S. E.; Watts, N.; Willett, P.; Bawden, D.; Fisher, J. D. Pharmacophoric Pattern Matching in Files of 3-D Chemical Structures: Evaluation of Search Performance. *J. Mol. Graphics* **1987**, *5*, 41-48.
(14) Brint, A. T.; Willett, P. Pharmacophore Pattern Matching in Files of 3D Chemical Structures: Comparison of Geometric Searching Algorithms. *J. Mol. Graphics* **1987**, *5*, 49-56.
(15) Sheridan, R. P.; Rusinko, A.; Nilakantan, R.; Venkataraghavan, R. Searching for Pharmacophores in Large Coordinate Data Bases and Its Use in Drug Design. *Proc. Natl. Acad. Sci. U.S.A.* **1989**, *86*, 8165-8169.
(16) Murral, N. W.; Davies, E. K. Conformational Freedom in 3-D Databases. I. Techniques. *J. Chem. Inf. Comput. Sci.* **1990**, *30*, 312-316.
(17) Motoc, I.; Marshall, G. R.; Dammkoehler, R. A.; Labanoski, J. Molecular Shape Descriptors. 1. Three-Dimensional Molecular Shape Descriptor. *Z. Naturforsch.* **1985**, *40A*, 1108-1113.
(18) Bohacek, R. S.; Guida, W. C. A Rapid Method for the Computation, Comparison and Display of Molecular Volumes. *J. Mol. Graphics* **1989**, *7*, 113-117.
(19) Weiner, P. K.; Langridge, R.; Blaney, J. M.; Schaeffer, F.; Kollman, P. K. Electrostatic Potential Molecular Surfaces. *Proc. Natl. Acad. Sci. U.S.A.* **1982**, *79*, 3754-3758.
(20) Náray-Szabó, G. Electrostatic Complementarity in Molecular Associations. *J. Mol. Graphics* **1989**, *7*, 76-81.
(21) Náray-Szabó, G. Electrostatics in Computer-Aided Drug Design. *Int. J. Quantum Chem., Quantum Biol. Symp.* **1989**, *16*, 87-99.
(22) For a nonelectrostatic-based approach to lipophilicity see: Furet, P.; Sele, A.; Cohen, N. C. 3-D Molecular Lipophilicity Potential Profiles: A New Tool in Molecular Modeling. *J. Mol. Graphics* **1988**, *6*, 182-189.
(23) Since there are no matches for the "brute force" procedure to operate on, the CPU time required for the second pass in this case is due to "overhead" in setting up the appropriate loops.
(24) Spivak, C. E.; Waters, J.; Witkop, B.; Albuquerque, E. X. Potencies and Channel Properties Induced by Semirigid Agonists at Frog Nicotinic Acetylcholine Receptors. *Mol. Pharmacol.* **1983**, *23*, 337-343.
(25) Mohamadi, F.; Richards, N. G. J.; Guida, W. C.; Liskamp, R.; Lipton, M.; Caufield, C.; Chang, G.; Hendrickson, T.; Still, W. C. MacroModel—An Integrated Software System for Modeling Organic and Bioorganic Molecules Using Molecular Mechanics. *J. Comput. Chem.* **1990**, *11*, 440-467.
(26) Behling, R. W.; Yamane, T.; Navon, G.; Jelinski, L. W. Conformation of Acetylcholine Bound to the Nicotinic Acetylcholine Receptor. *Proc. Natl. Acad. Sci. U.S.A.* **1988**, *85*, 6721-6725.
(27) Spivak, C. E.; Waters, J. A.; Aronstam, R. S. Binding of Semirigid Nicotinic Agonists to Nicotinic and Muscarinic Receptors. *Mol. Pharmacol.* **1989**, *36*, 177-184.
(28) Peet, N. P.; Leutz, N. L.; Meng, E. C.; Dudley, M. W.; Ogden, H. M. L.; Demeter, D. A.; Weintraub, H. J. R.; Bey, P. A Novel Synthesis of Xanthines: Support for a New Binding Mode for Xanthines with Respect to Adenosine at Adenosine Receptors. *J. Med. Chem.* **1990**, *33*, 3127-3130.
(29) Herdlklotz, J. K.; Sass, R. L. The Crystal Structure of Acetylcholine Chloride: A New Conformation for Acetylcholine. *Biochem. Biophys. Res. Commun.* **1970**, *40*, 583-588.
(30) See, for example: Still, W. C.; Tempczyk, A.; Hawley, R. C.; Hendrickson, T. Semianalytical Treatment of Solvation for Molecular Mechanics and Dynamics. *J. Am. Chem. Soc.* **1990**, *112*, 6127-6129. Gilson, M. K.; Honig, B. The Inclusion of Electrostatic Hydration Energies in Molecular Mechanics Calculations. *J. Comput.-Aided Mol. Des.* **1991**, *5*, 5-20.
(31) CP is available from QCPE.

Chemsits' Use of Libraries

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Interviews have been conducted with a number of chemists, predominantly in the United States, in industry, government, and academia. Chemists working in some areas of the science depend heavily upon the literature, and such chemists show a uniformity in their work patterns which transcends the differences in their organizations. There are striking similarities in their need for literature and in the practical arrangements that they have made for access to it.

INTRODUCTION

The relationship of scientists to their literature is well-documented. As a professional group, scientists are strongly dependent on the work of their colleagues and predecessors. Unlike law, a field which also is heavily dependent on its literature, science depends on conferences, workshops, and informal networks as well. All these secondary means of generating literature are within the public domain, and all are capable of being accessed by workers in the various scientific fields.

It has been noted that in general, scientists are very aware of their literature. The chemists interviewed are frequent and proficient users of their own literature. They view this as an accomplishment. Examination of some university undergraduate catalogues shows that generally instruction in the use of the chemical literature is not taught by the chemistry department to its majors in a separate course. (The undergraduate catalogues of 12 colleges were examined. Each was the home institution of an interviewed chemist. Only one mentioned library involvement in the catalogue. That one specified the use of library materials in the senior thesis course.) However, when asked, practically every chemist who teaches will make a point of saying that he/she incorporates the literature in the courses taught and brings classes to the library consistently. This is vital since chemistry and its allied fields generate a considerable portion of the scientific literature. It is a reflection of the prominence of chemical and related industries in society.

One constant complaint of the working scientist in the pressure of the need to keep up with an ever-growing literature. Chemists, having the largest literature to cope with, will list their library time as a major component of their professional lives.[1] However, within the large discipline of chemistry in general, a particular group of chemists in the special fields that might be termed "theoretical chemistry" tend to stress their dependence on literature and libraries. Computational chemists who work in physical organic chemistry or molecular design are such specialists.

Such chemists can be found in pharmaceutical companies, government, universities, and chemical companies manufac-

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turing agricultural materials such as pesticides. Since these professionals can be grouped by the kind of chemistry they do and this chemistry involves intensive use of chemical literature, we attempted to determine whether there are similarities in the library habits of these individuals. Are there patterns seen across the specialty? Do these chemists use the same tools, employ the same methods, and have the same demands on collection and library personnel? How central is the library in the daily function of chemists at a particular institution? What is the level of satisfaction with the library, and what factors are responsible for that level?

METHOD

We intended to examine work habits of a group of people with the same or related research interests, and we interviewed 56 chemists who are currently working in computational chemistry and related fields. The choice of speciality narrowed the possible array of independent variables. Those interested in pure chemistry tend to be physical chemists or organic chemists using physical chemistry; while those who are interested in bioactivity are most often medicinal or environmental chemists.

This survey of chemists was undertaken with several objectives in mind.

1. Are these similarities in the working methods of such chemists?
2. Do they rate the same tools as their primary tools?
3. Do they have the same requirements of their libraries or of their librarians?
4. How much control of the collection and its arrangement by the library staff do they consider optimal?
5. What other arrangements are entered into as part of the chemists' efforts to keep abreast of the field?

To collect answers to these questions and to determine the level of satisfaction with library services, we interviewed a number of such chemists both at their institutions and at professional meetings where they were presenting current work. This served to establish them as currently working professionals in their established field of interest. The rationale for using interviews was that written surveys are limited to the questions asked, an interview will elicit response that is useful and may have not been included in the questionnaire. The direct approach also ensured response. No chemist selected as a source of information for this survey refused to be interviewed.

Two people in the survey were used as reporters for two different institutions. One had recently moved from one to the other; the second chemist was, at the time the survey was conducted, on sabbatical. He therefore reported on both his home institution and that at which he spent the sabbatical.

All of the interviewed chemists are at the Ph.D. level. While chemists holding doctoral degrees are a group comprising less than half the total number of employed chemists,[2] they are the ones who are directing research efforts in industry, government, and academic institutions. The subjects were asked a number of questions which were designed to elicit responses that indicated the researcher's involvement with library, his or her method of use of the literature, and the level of use of newer library technology in the library and at a distance. Some chemists access the library collection by means of the university or corporate in-house network.

The chemists were chosen as representatives of a number of different situations. These variables are

A. Six chemists are in industry.

B. One is a self-employed consultant to his former company. He is counted as an industrial chemist.

C. One is a research associate working at a non-Ph.D.-granting academic institution.

D. Three work for the U.S. government.

E. Twelve are from institutions outside the United States; of these, three are from non-English speaking countries.

F. Among the U.S. academics, 10 are in institutions that have largely or wholly undergraduate student bodies and no Ph.D. program in chemistry. (Several interviewed chemists who have been counted as belonging to Ph.D.-granting institutions are employed by City University of New York. The University as a whole grants the Ph.D. in chemistry. However, doctoral students are based at individual colleges. Each individual college in both enrollment and outlook is an undergraduate institution.) The remaining number are in Ph.D.-granting institutions. They range from assistant professor to full professor and full professor emeritus.

The object was to attempt to quantify a fairly subjective response on the part of a sample to the library. All the respondents identified "Library" as an entity that was essential to them in their work. Its use was not a sometime thing with any respondent. The questionnaire was designed following the guidelines suggested in *Measuring Academic Library Performance*.[3]

The questions asked the chemists were based on the following list.

1. Are you employed by
   a. a university or college
      i. how large is your department (faculty and students)
      ii. highest degree granted by your institution
   b. industry
   c. government
2. Is your library departmental or central?
3. Who selects monographs and periodicals for your library?
4. What fraction of your choices of monographs and periodicals does the library purchase?
5. How often do you use the library?
6. What do you use most often: books, periodicals, indexes, or (abstracts)?
7. Does your library have CD/ROM capability?
8. Do you use it?
9. How do you maintain current awareness?
10. Do you have access to online searching?
11. Do you have direct access to online searching or does your library do it for you?
12. Which databases are searched?
13. Do you use interlibrary loan?
14. How rapid is turn-around?
15. What areas of strength does your library have?
16. What areas of service in your library would you improve?
17. Is the library staffed by professional librarians?
18. Do you use a library other than the one at your workplace?
19. If no. 18 is yes, is this use occasional, frequent, always?
20. Why?
21. What library or libraries do you use?

The last question almost invariably produced a discussion of both the home library and the other installations used and the level of service encountered there.

Tables I–III summarize the results of the survey.

RESULTS

The sample is felt to be representative of the chemists working in this area of chemistry. The study looked at people who work in a number of different settings and who have varied expectations concerning output. The sample is not large enough to allow meaningful statistical analysis, but we can observe significant trends. In addition to the obvious, unsolicited response from all the chemists interviewed that they consider the literature as a paramount tool in their work, all of them use *Chemical Abstracts*, and for all but one it is the

Table I. Library Quality Assessment

	academic libraries		
	Ph.D.-granting	non-Ph.D.-granting	industry and government
overall assessment			
good	22	3	9
adequate	10	4	1
poor	3	7	
input in purchasing			
all	19	0	5
most	13	4	5
some	7	5	
none	2	4	
contacts/week			
≥2	20	2	9
<2	19	8	1
library location			
dept or division	20	1	2
area within main	7	2	8
undifferentiated	11	8	

Table II. Use of the Literature

	academic libraries		
	Ph.D. institution	non-Ph.D. institution	industry and government
personal online use	18	6	5
colleague online use	16	3	2
SDI by library	8	0	6
use of indices not CA or SCI	5	4	6

Table III. Use of Other Libraries

	academic libraries		
	Ph.D. institution	non-Ph.D. institution	industry and government
no ILL use	10	4	2
return time >1 wk	19	7	2
personal visits	23	18	7
no. of visits >1/month	9	9	1

first index used. All those interviewed consider the periodical literature of highest importance; monographs, while very important, are not as critically sought after as are periodicals. One chemist said it very simply, "Reviews go out of date; data in the periodical literature is forever".

Chemists also use *Science Citation Index* and for almost all it is the second indexing tool. They expect to find both *Science Citation Index* and *Chemical Abstracts* in hard copies in the library. They are for the most part searching manually. While machine searching is done, they "feel more comfortable" with the paper copy. Several said that they learned to use the literature effectively by doing hand searching and that it was familiar and reliable. They used machine searching to make sure that they had not missed anything. They were proud to report their own manual searching expertise.

The people who are happiest with machine searching are either doing it themselves, usually in the chemistry office, or having a chemist-colleague do it for them. The charges for the machine searches are paid for out of department or grant budgets. These expenses are not considered extraordinary. The chemists who use CA Online are satisfied with their own performance; they feel that they do better than do the librarians who are also doing searching. When questioned about the level or depth of coverage of the average online (or CD) search, the chemists believed that they were best able to select the few pertinent articles that they wanted. As the people on a particular "cutting edge", they are sure that they can spot what they will need. They seldom expect many hits. They usually expect to find related materials and background and will search diligently to make sure that nothing of significance is missed. This is vital to them since they want to make sure that if they are involved in a specific piece of research, no one has "scooped" them. One complaint that is voiced about librarians as searchers is that they tend to retrieve far too much.

Interlibrary loan is important to everyone.[4] It is accepted by everyone working in this field that it is impossible for any library to have everything. The chemists are not asking that the library own every possible periodical that they might need. They do expect that if they are going to be using periodicals in a specific field, that those periodicals appear farily quickly. They expect to change the periodicals list annually. They also expect delivery of xerox copies of specific articles as soon as possible. The optimum seems to be within a day or two. This level of service is available to some. Those who reported an average of 2–3-week delays in receipt of interlibrary loan were most unhappy about it. They are aware of better service in other institutions. They are also the people most likely to find other sources of library materials thereby eliminating all but a small fraction of their requests for journals not held by the home library. Once they begin to use another library on a more than occasional basis, they tend to use it for all but the most trivial of their library needs.

The chemists interviewed are aware of the cost of the library materials. They are perhaps not aware of the great difference in the cost of a personal subscription as compared with an institutional subscription but they do have a great awareness of the tendency for price escalation, particularly that of periodicals produced by commercial publishers.

As a group, this sample of chemists tend to provide support for their own research. They buy books and journal subscriptions both out of their own funds and with whatever grant and departmental money they have available. The chemists interviewed who were critical of their home libraries were most often dissatisfied with the response (or lack of it) to requests they made for purchases.

This does not seem to be a problem in nonacademic settings. In both industry and government—more so at the former than the latter—if the research department wants it, it appears as soon as possible. This is very similar to the usual mode of operation in medical libraries. (Private communication with Judith Topper, Librarian, Cabrini Medical Center, New York.) The industrial chemists interviewed were all very pleased with their in-house libraries. The librarians were professionally trained as both chemists and librarians. In some places, the librarian-chemists were doing SDI and searching exclusively. While the computational chemists were doing some—or even all—of their own searching, others in the company were relying on the chemist-librarians as searchers.

The industrial chemists were also the ones that were most anxious to have complete information and to have it immediately. They were quite willing to have a pertinent piece of information either read to them over the telephone or have it sent by FAX. In all their interlibrary transactions, they counted time as the most important factor. They expected to have all their support materials in the library. When they change research projects, or begin on a new aspect of a continuing problem, they consult with the library and together design a start-up collection to support the new area of interest. Considerations of budget are dependent on allocation and subject to change, depending on long- and short-term projections.

Those chemists that work for government are very conscious of the budgetary constraints on their work and the purchasing capability of the libraries that serve them. They do have a great advantage however, in that their libraries are most likely to be buying materials which are subsidized and their libraries are also most likely to be government depositories. They do

very well in terms of value-for-money spent. The sample of government chemists interviewed all reported a slow response to requests for new titles. Since they are from different laboratories and each is representative of a group, we looked at them as more than a single-reporting unit. They all felt that service was good. Response from other government installations is also very good. While the sample of chemists includes very few who are in government, those surveyed felt that they are treated as "at home" when they do use the libraries at other government institutions. One chemist in the Washington, D.C., area, while using a library at an institution not his own, found that he needed a paper that neither his library nor the library he was using owned. The host library placed an interlibrary loan request for him and had it delivered to him at his institution in 3 days.

The questions about interlibrary loan also elicited much discussion. Those chemists who were happiest with the service were those who received the requested material in a matter of days. One, who is at a very large school and uses the service infrequently, put it as follows: "I want what I want now. Three weeks from now means that I'm following a cold trail. I haven't been sitting around for three weeks. If it has to take that long, I'll go get it myself." This is also the essence of the industrial and/or government chemist.

The largest group of interviewed chemists are academics. They are a group that takes research seriously; most are involved in teaching others both chemistry and how to do research. As a group, they are less likely to have chemically trained librarians. Several (none in the United States however) have librarians who are not trained as librarians.

A very sharp separation is noted between those institutions that are largely or wholly undergraduate and those that have large numbers of graduate and/or postdoctoral students. In this study, chemists who are working at undergraduate schools are least likely to be happy with their home libraries in terms of collection. Most are also critical of the library staff and services as well. Since most academic chemists work in such institutions and some obviously do maintain a significant level of research, it seemed reasonable to look at how they do library work when they are doing a significant portion of it away from home.

Almost all of those chemists who are researchers and work at schools that have limited library resources have other libraries that they use on a regular basis. These other libraries are almost always the ones closest to hand. Waiting time seems to be the determining factor. Therefore a quick trip to a nearby library where the researcher is fairly sure to find an answer is frequently seen as the best option if a quick telephone call is not a possible source of information.

When asked to elaborate on level of satisfaction with the home library, a significant number (34 of 56) of the chemists studied noted that they were quite pleased with the library service. This satisfaction was made up of a number of factors. Those fortunate enough to have librarians who were chemically trained mentioned that first. It was with such librarians that they had greatest rapport and understanding of their needs. They felt that such librarians were also most likely to "buy correctly". They also know that almost all of the needs of their clients are for information in the periodical literature or in conference proceedings.

Interestingly, the location of materials in the library was rated as even more important than the knowledgeability of or the rapport with the librarian. Many respondents have departmental libraries. Of all the academics interviewed, these respondents were the most pleased with the library even if they do not have extensive collections. They have greatest control of what they do have, can use it with a minimum of effort, and have greatest and most effective contact with the librarian on-site. They expressed the feeling that this on-site librarian was their advocate and representative.

In those libraries where the chemistry library or the area library (i.e., chemistry or physical science) was an autonomous unit, the level of satisfaction was higher than in those institutions where the library was central. Satisfaction was at its lowest level in those libraries where the periodicals collection was arranged alphabetically in a central library and at a distance from the monograph collection. Several of the interviewees were at institutions that have this type of library.

While no one interviewed likes using microforms, most will accept their space-saving rationale. Complaints about the lack of functional copiers was frequent. This is apparently a universal problem. All the interviewees are willing to deal with microforms if they produce a black-on-white readable copy. Many feel that the reality is nowhere near that ideal.

The copier is a fixture in every library. Those chemists who use the library extensively are most pleased with the copying arrangement if they can (1) make their own copies using the departmental by-pass on the public copiers or (2) send a student aide to the library to make copies either using a departmental by-pass arrangement or a departmental charge account.

The use of other libraries varies considerably. Even chemists at institutions with very well stocked libraries will on occasion need something that their library does not own. That does not surprise them. They do expect that this is an occasional occurrence rather than the normal. These people, such as the NIH (National Institutes of Health) chemist who finds his home library just middling in straight chemistry, will accept that without a problem. He is close enough to another library that does have more of the journals of interest to him to use as an alternative source. He does not consider that his own institution's library is providing poor service or collection development. There are other research chemists that use alternative libraries for all but the most basic journals. Their attitude toward the entirety of the home library–collection, personnel, and service—is most likely to be negative.

CONCLUSIONS

In our sample, the chemists are very sure of themselves and want little or no library help. When asked directly if this was indeed their attitude, most agreed that it was. One interviewee stated that "... I don't want the librarian as a partner in my research. I know more about my research than anybody else." But, almost all the chemists interviewed expect that the monographs, serials, and periodicals collections in their home institutions will fill almost all of their demands. If this is to happen with a reasonable success rate, chemists and librarians must talk to each other on a constant and meaningful level both within a given institution and in conjunction with representatives who are at other institutions.

The cost of library materials is considerable. The demands for new serials and specialized monographs and journals are increasing as these products appear. Nontraditional formats (i.e., CDs or hypertext) are a fact of life for both the chemists, who sometimes see these factors as obstacles in their quest for data, and the librarians who try to help them.[5] Chemists are not librarians nor need librarians be chemists. In those institutions where there is general satisfaction with the library, there is considerable dialogue and discussion on a constant basis. Several chemists mentioned the annual review of orders for periodicals, annuals, and monographs by the entire chemistry department or a large committee made up of faculty and librarians.

Nevertheless, there is a significant group of research chemists who are unhappy with their libraries. Given the demands for services which are apparently available for some,

it seems that there is a magic point in every dissatisfied library work when he/she decides that the home library is a hostile environment. These people leave. They continue to do their work, but they do it elsewhere.

This has enormous significance for many institutions. It is no secret that even modest chemistry collections are expensive.[6] If they are under-utilized because the on-site users are going elsewhere, both the library and its disgruntled clients are at a disadvantage. From the chemists' point of view, that library may be seen as having failed in its mission. The library, on the other hand, may look upon the chemists as ungrateful and demanding. In the interests of improved service in an era of tight budgets and simple efficiency, it would be useful for some libraries to compare their methods with those of the libraries those whose users feel that they are very well served.

REFERENCES AND NOTES

(1) Maizell, Robert E. *How to Find Chemical Information*; John Wiley & Co.: New York, 1987; Chapters 4 and 10.
(2) Peters, Marion C. Chemistry. In *Scientific and Technical Libraries*; Pruett, Nancy Jones, Ed.; Academic Press: New York, 1986; Vol. 2.
(3) Van House, Nancy A.; Weil, Beth T.; McClure, Charles R. *Measuring Academic Library Performance*; American Library Association: Chicago, 1990.
(4) Rollins, Stephen J. Document Delivery. In *Scientific and Technical Libraries*; Pruett, Nancy Jones, Ed.; Academic Press: New York, 1986; Vol. 1.
(5) Echelman, S. T. Why Do Academic Libraries Get Such A Bad Rap?. *Libr. J.* **1988**, *113* (Oct 1), 39-41.
(6) Dionne, R. J. Science Libraries At a Crossroads. *Am. Sci.* **1988**, *76*, 268-272.

Deciphering the Information Content of Chemical Formulas: Chemical and Structural Characteristics and Enumeration of Indacenes†

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Constant-isomer series for indacene-related compounds are presented. These results illustrate the generality of the previously developed algorithms and associated concepts. The indacenoid constant-isomer series exhibit a repetitive ...abac... isomer number sequence. The constant-isomer series with the same isomer number have a one-to-one matching in the symmetry distribution of their membership.

INTRODUCTION

While numerous enumerations of benzenoid isomers have been reported (only a representative list is given herein),[1-3] very little work has been done on other polycyclic hydrocarbons.[4,5] Polycyclic hydrocarbons related to indacenes represent an important subgroup of the polycyclic group of pyrolytic pollutants,[6-8] and the enumeration of these isomers is the subject of this investigation. Indacene-related polycyclic hydrocarbons (indacenoids) have two pentagonal rings among otherwise hexagonal rings. Indacenoid constant-isomer series will be presented. The formula periodic table for indacenoid hydrocarbons and the enumeration studies provide the framework for understanding the limits of what we know and can learn about indacenoids. This epistemology represents an important goal in deciphering the information content of chemical formulas.

Over 25 indacenoid hydrocarbons isomeric with benzenoids have been synthesized.[9] Indacenoids that are not isomeric to benzenoids will be discussed here. Indacenoids are expected to be strained and frequently nonplanar. An indacenoid of 50 carbons is offered for sale by a commercial vendor.[10] A brief view of some noteworthy chemistry of indacenoids will be presented.

Our general approach to the enumeration of polycyclic aromatic hydrocarbons involves construction of an appropriate formula periodic table and using the aufbau principle and excised internal structure concept (see below) to enumerate the isomers found on the edges of the corresponding formula periodic tables. In this way, we have successfully enumerated even- and odd-carbon benzenoids having unique characteristics. In both cases, constant-isomer series have been found where the isomer numbers alternate between singlet and doublet occurrence, and there exists a one-to-one matching in the symmetries between the member compounds with the same isomer numbers.[11] The isomer numbers have the same sequence of values between the strictly peri-condensed and the total resonant sextet subsets and between the monoradical, diradical, triradical, etc. subsets.[12,13]

In addition, this approach has shown that constant-isomer series also exist for fluorenoids/fluoranthenoids having one pentagonal ring among hexagonal ones.[5] Again these constant-isomer series exhibited isomer numbers that alternate between singlet and doublet occurrence and those member compounds belonging to series with the same isomer number exhibit a one-to-one matching in their symmetry distributions. We demonstrate here that indacenoid hydrocarbons also have constant-isomer series which follow the above topological paradigm, i.e., they have isomer numbers that alternate between single and pairwise occurrence with a one-to-one matching in the symmetries of the member compounds that have the same isomer numbers.

RESULTS AND DISCUSSION

Excised Internal Structure Concept. If a conjugated hydrocarbon is encircled by a perimeter of carbon atoms with the appropriate number of hydrogens, this process is described as *circumscription*. The reverse process (*excision*) leads back to the excised internal structure. A polycyclic conjugated hydrocarbon may not have two or more bay regions if it is to be circumscribed. All constant-isomer series are generated by successive circumscription, are strictly peri-condensed (if the number of rings $r > 2$), and correspond to formulas on the left-hand edge of the relevant formula periodic table. A constant-isomer series consists of compounds which, when circumscribed as described here, give at every step compounds

† Dedicated to former Editor Herman Skolnik, who contributed significantly to the area of chemical information.

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