Indexing and Index Editing at Chemical Abstracts before the Registry System

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Abstract

Indexing and index editing at *Chemical Abstracts* before the CAS Registry System (and during its development), while based on sound principles of documentation, were tedious, labor intensive, and error prone. Images and recollections from those times provide an interesting contrast to our current reliance on hardware and software that generate names from structures and vice versa. Systematic nomenclature was virtually essential for vocabulary control in printed subject indexes, and it remains the gold standard for written communication. However, today's best computer-based systems and contemporary software permit users to search under whatever names they prefer. While the efficiency of the new systems should be celebrated, it is also worthwhile to reflect on the "romance" inherent in the production of indexes in the early days of *Chemical Abstracts.*

Originally titled "John Henry Was an Indexing Man (or Woman)," my presentation deliberately compares early scientific information handling with industrial labor and a comparable transition to mechanization. As one who was privileged to work at the Chemical Abstracts Service (CAS) from 1962 through most of 1965 (when I resumed graduate studies), I will reflect on some of the features of this transition period, particularly the effort and skill required before computers made life much easier. In addition, I intend to comment on some of the implications of the technological developments that started during that time and continue to offer promise and pitfalls.

From its inception in 1907, indexing procedures for *Chemical Abstracts* were based on well-established techniques derived from documentation and library science. General subject headings in *Chemical Abstracts* conformed readily to the established traditions. However, chemical substances—especially the burgeoning number of organic compounds and their derivatives—required special treatment. Among other things, this involved the establishment of separate departments in *Chemical Abstracts* for indexing and editing these special entries because it became apparent that greater accuracy and precision would be attained if different people were responsible for the two operations.

These were the last years of the second generation of computers, and CAS had just added an IBM 1401 to its collection of Hollerith card–based electronic data processing equipment. Mini- and microcomputers were several years in the future, and mainframes were cumbersome beasts that typically used six-bit bytes. Without going to a lot of trouble, one obtained printed output conforming to the notorious "IBM Gothic," with its upper-case type, decimal numerals, and a handful of punctuation marks. It was also the era during which John Glenn first orbited the Earth, John F. Kennedy was assassinated, and Lyndon Johnson defeated Barry Goldwater for the U.S. presidency.

To offer a more immediate perspective, *Chemical Abstracts* and its indexes were still being produced using hot type in 1962, and the third generation of computers did not arrive until 1964, with the introduction of the IBM 360 series of machines and their eight-bit bytes, direct-access disk storage, and much greater speeds (Figure 1). Things changed quickly after that. In fact, it is now hard to imagine just how labor intensive most procedures were before that major transformation in information technology took place.

The Old "New Building"

When I arrived as a young assistant editor in the Organic Index Editing Department in 1962, I found CAS

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located in a four-story building on the north side of the Ohio State University campus. This building was originally a three-story structure built specifically for CAS in the mid-1950s. A fourth floor was added in 1960 to accommodate the staff, which had grown from a relatively small number of individuals located in the university's Chemistry Building, to approximately three hundred people (Chemical Abstracts Service, n.d.). The administrative offices were on the second floor, general indexing and editing occupied the third, and both the Organic Indexing and the Organic Index Editing departments were on the top floor. Research quarters were relatively small and on the lowest level, presumably because of the heavy equipment housed there. That is also where the vending machines were located, and staff could enjoy them during each of two fifteen-minute breaks, one in the morning and another in the afternoon.

Figure 1. *Milton Harris, Fred Tate, and Dale Baker (left to right) inspect a newly installed IBM 360/40 computer (1967).*

Early Research and Development

G. Malcolm Dyson, having arrived from England in 1959, would soon leave CAS, but in 1962 he was still in charge of research and development. Dale Baker has described the circumstances that occasioned the purchase of the IBM 1401 computer. Dyson had invited IBM's Hans Peter Luhn to visit and discuss his keyword-in-context indexing technique. During this visit CAS realized that it did not yet possess even a primitive computer, and this discovery prompted the first of several successful grant applications to the National Science Foundation, which resulted in the development first of *Chemical Titles* and ultimately of the Registry System (Baker, 1998).

Dyson, however, is remembered for having succeeded in lobbying for his system of linear notation, which won the approval of the International Union of Pure and Applied Chemistry (1961). This triumph over the more popular Wiswesser notation was something of a pyrrhic victory since linear notation ultimately would never be important to CAS. Other organizations, especially the Institute for Scientific Information, would go on to use Wiswesser notation, and it became an industrial standard for those who needed linear notation in their work (Davis & Rush, 1974a). However, the principal reason that CAS did not use either system was that during the early 1960s a young mathematician named Harry Morgan developed the famous algorithm that led to the Registry System (Morgan, 1965; Davis & Rush, 1974b).

During this period Michael Lynch and other colleagues also began important work on the production of articulated subject indexes as well as substructure searching (Barnard, 1993; Willett, 1998). Lynch's paper (M. F. Lynch, personal communication, 15 November 2002) expands on events during this era; moreover, he makes it clear that the Morgan algorithm was actually a revised version of the Gluck algorithm developed at DuPont. David Weisgerber (1997) has described the era following the establishment of the Registry System very well.

Morgan and his colleagues knew that the first step in indexing organic compounds typically involved drawing chemical structures in two dimensions, and he realized that a connectivity table could be used to generate unique representations of the compounds. The CAS administration, which by then included Fred Tate, the associate director, conducted internal seminars and invited staff participation. Topics ranged from Morgan's ideas to presentations of how payroll would be moved from American Chemical Society (ACS) headquarters to Columbus, Ohio. However, the concept of the incipient Registry System was paramount. Morgan, who had earned his B.S. degree in mathematics from Capital University in Columbus, was very approachable. I vividly remember a conversation with him in which I pointed out that chemical molecules were really three-dimensional in spite of how chemists usually drew them. He responded, "I know, but that's too hard." Stereochemistry, aromaticity, and peculiarities such as keto-enol tautomerism were a challenge then and sometimes now (Davis, 1966).

Administration and Benefits

Evan J. Crane had retired in 1958, and his longtime assistant, Dale Baker, assumed the position of director.

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He and Fred Tate ran the show. Dale had ultimate responsibility for everything, but it was apparent that he enjoyed a special relationship as liaison with the ACS headquarters in Washington, D.C., while Fred was primarily responsible for R&D and other operations in Columbus. Fred adopted the habit of looking out a second-story window at starting time. Newcomers felt threatened, but the rest of us were merely amused by his performance. Adept with carrot as well as stick, Fred, who assumed that professional staff would be members of ACS, encouraged us to join the American Documentation Institute (now the American Society for Information Science and Technology). At that time it was possible to join local chapters without joining the national organization, and I was one of a number of new staff members who joined the Central Ohio Chapter. We were rewarded with interesting presentations ranging from edge-notched card applications to Bell Telephone Laboratories' early attempts at computer-based voice recognition.

Production of the indexes required overtime from some of the staff; however, it was entirely voluntary. Ongoing commitments of overtime of 10 to 20 percent were common—especially while annual and collective indexes were being prepared simultaneously. Although less common, 30-percent overtime was also invoked occasionally and showed how serious and labor intensive the operations had become. In any case employees who could afford the extra time welcomed the chance to make more money.

Middle management was personified by Ferd Wetsel, the managing editor, and the various department heads. David Whittingham was in charge of the Organic Indexing Department, along with his assistant and eventual successor, Paul Schwartzentruber. Mary Magill headed the Organic Index Editing Department with her assistant, John Stone, who was in charge of formula index editing, a special assignment to be discussed later. "Structure drawers" (as they were then called) were part of the Organic Indexing Department and subsequently became known as "formula indexers" in recognition of their special status. Arveta McKim headed this group for a long time.

Leonard T. Capell, who pioneered the *Ring Index* with Austin M. Patterson, was still on staff but would soon retire. During this period he published a second edition of the *Ring Index* with Donald F. Walker (Patterson, Capell, & Walker, 1960). Capell and Walker assisted indexers and editors alike with questions related to naming ring structures, especially for important classes of compounds like alkaloids, terpenes, and steroids, a task eventually assumed by Casimir Gladys.

Organic indexers, editors, and their support staff were all close to one another on the fourth floor, which fostered a friendly atmosphere and cordial relationships. Rank and attained degrees, while important, were not overly emphasized, because what mattered was whether one could do the work. In fact, Ph.D. chemists sometimes failed to make the grade and left, not because they were incompetent chemists but because they lacked editorial or proofreading skills—especially those requiring nearly instant recognition of discrepancies between chemical names and their formulas as well as other errors in index entries. I was an oddball, having a B.S. in chemistry with a combined minor in mathematics and physics, plus a peculiar mix of thirty-eight semester hours of graduate credit in chemistry and toxicology. After proving myself worthy, I was given credit for a master's equivalency, a nice raise, and an outside office, a perquisite described below. In addition to formula index editing, I was given the task of trying to manage references for the infamous "starred" entries—those for which neither a name nor a formula could be determined. Such entries were called "starred" because they always carried an asterisk in the subject indexes.

Going into administrative work was one avenue for advancement at CAS during this era. The other way was through scientific and technical expertise, however obtained, so that an individual could advance from assistant to associate editor. Among those who chose the second route, some were clearly more equal than others, and rank was indicated by whether one had an office with an outside window. Competence was the ultimate criterion for success. Nevertheless most senior staff held Ph.D.s or master's degrees, or their equivalent. All professional staff members enjoyed good perquisites. One-month vacations were the norm, and up to two weeks of these vacations could be taken either as single or half days. Unless a department head had a compelling reason to countermand such a request, he or she gave it without question. To say this was unusual at the time is an understatement. The ultimate perquisite for professionals, however, was a corner office with two outside windows. This extravagance was reserved for department heads and senior management.

Support Staff

Librarians and Bibliographers

Under the able direction of James L. Wood, the library staff provided professional bibliographic support for

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indexers and editors alike. In addition to the tasks normally associated with library activities, staff was of considerable help in keeping track of the patent literature.

Alphabetizers and Stenographers

There were two kinds of clerical staff: "alphabetizers," who did what their title implied, sorting three-by-five cards into the alphabetical (and other) order prescribed for the indexes; and stenographers, skilled and specially trained typists who received recorded dictation from the indexers. Alphabetizers occupied the open space outside the offices of professional chemists (Figure 2). To help with sound reduction, stenographers had individual offices.

Stenographers were extraordinary and obviously had to know how to transcribe passages involving terms that the average high-school graduate might find difficult, even with a modicum of college education. However, alphabetizers were truly special. The rules for sorting involved far more than knowing the alphabet. Indeed, it required memorizing such things as this: for inverted entries such as "Tridecane, 6,7-bis(3,3-dimethylbutyl)-3,4,9-trimethyl-," "d" comes before "m" to determine alphabetical order rather than "b" before "t." Moreover, numeric prefixes determined alphabetical order only when within curves or brackets, and whenever Greek letters appeared in a series of locants for substituents, they had to be placed following roman letters but before numerals. Also to be considered for complex groups were Greek as well as Latin prefixes. Everyone had to deal with bis-, tris-, tetrakis- as well as with di-, tri-, tetra-, and so on. Mercifully, braces ({ }) were discontinued after the Fifth Decennial Index. They were considered an unnecessary complication, even though they did help to resolve the issue of "what went with what."

So the clerical staff took great pride in their work, and they often caught mistakes that might otherwise have eluded the chemists, who understandably tended to focus on the technical aspects of the entries. The senior clerical staff also read galley proofs when they came back from the printer. Staff members were instructed to confer with chemists when they found a technical name that looked radically different from the norm, and they performed tirelessly and were integral to a collegial effort that benefited the entire enterprise.

Before Computers Were Instrumental

As mentioned, in the early 1960s *Chemical Abstracts* and its indexes were still produced by using hot-type methods. Most abstractors were not in-house employees but instead were practicing chemists in the field who volunteered their contributions. At that time over three thousand of them read and abstracted the primary literature and were rewarded in two ways: first by being acknowledged on the masthead, and second by receiving the grand sum of 10 cents per printed line. An additional incentive (touted by CAS, of course) was that abstracting represented a good way of remaining current in one's field. A few abstracts were prepared in-house, typically those involving abstruse technical or unusual foreign-language materials.

Indexing

General and inorganic entries were assigned to the "third-floor" group, while the bulk of the chemical compound entries were handled by "fourth-floor" formula indexers (structure drawers), who looked at the copies and abstracts of all articles before drawing the structures of the compounds. They also verified the bibliographic information and recorded all relevant information pertaining to the compounds or substances discussed in the original papers. Once they had completed their work, they handed off items to the senior organic indexers. These individuals accepted responsibility for supervising the work given them, and when they were sure that the information was accurate, they proceeded to write or dictate the actual index entries.

Indexers were responsible for what professional catalogers call "main entry," which is where people ideally would expect to find things in a catalog or index. As in any good indexing service or library of the time, CAS maintained a compilation of three-by-five cards, called the "master file" of cross-references. In it were the synonyms under which a chemical compound might be found, along with information about its preferred name.

Figure 2. *The alphabetizers.*

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Even in the early 1960s there were well over ten thousand cross-references, and the number of ambiguous names, identified in the printed index by asterisks, kept growing. This was largely because of the proliferation of generic pharmaceutical names, but thanks also were owed to patent lawyers, whose job sometimes involves deliberately obfuscating proprietary information.

Index Editing

After stenographers (or sometimes the indexers themselves) produced the three-by-five cards, the resulting data were passed along to alphabetizers. The "cards" actually were made of paper and were color coded, first to identify the *Chemical Abstracts* volume with which they were associated and second to indicate whether they were intended for the subject or the formula index. Each annual volume had unique subject and formula colors that were recycled after a few years so that they would not be confused within a given collective index period. Volume numbers were printed on the card stock, but color codes were quite helpful—except when they corresponded to volumes in the preceding collective index that was being edited at the same time!

Subject and formula cards were then interfiled for a pre-edit, which fulfilled two functions: making sure that empirical (molecular) formulas conformed to the names given them in the subject index, and providing an opportunity for new employees, then called formula index editors, to establish themselves as worthy of future employment. One quickly learned a few tricks of the trade. For example, editors looked for how many nitrogen atoms were present in the compound. If there was an odd number, then the number of hydrogen atoms should also be odd (absent other tri- or pentavalent atoms such as phosphorus). Needless to say, such tricks were necessary but not sufficient to guarantee success. They were helpful, however, for initiates.

After the pre-edit, separate subject and formula edits were done. The cards were separated and distributed to different senior editors whose responsibilities corresponded to the tasks implied. When discrepancies were found, senior editors would put paper clips on the cards and send them to junior staff members for correction. Usually the issue was easily dispatched, but further research was sometimes needed. Depending on the problem, junior editors looked up the original documents, spoke with the senior editors involved, sought out the indexers, or in extraordinary cases went to the Nomenclature Department—that is, spoke with a colleague in an office about twenty feet away.

An interesting and innovative procedure involved the insertion of "see from" references. These were the "opposite" of cross-references and were used to alert editors to whether or not the references were needed. These cards were always color coded pink, were called "the pinks" by everyone, and had to be interfiled manually by the clerical staff in accordance with the same alphabetizing rules used for other entries. Cross-references were printed if, and only if, entries for those particular names appeared.

Proofreading

After the pre-edit and subject and formula editing, cards were bound with string and sent to a printer, who prepared galleys. The next few weeks were spent reading these galleys, comparing them with the original cards whenever something was unclear. Senior editors read the galleys and corrected obvious typos. When there was a serious discrepancy, they sent both the galley proof and the original cards to junior staff members to determine what was wrong. Subject and formula indexes were handled separately but considered jointly, which meant that assistant editors could expect to receive problems from either quarter, often simultaneously. Sometimes either a formula or a subject problem's solution was self-evident and made correcting the other entry easy. However, it was not always so, and editors—junior and senior alike—cooperated extensively, showing considerable patience and ingenuity in resolving inconsistencies.

When they were ready, galleys were returned to the printer, who made corrections and then prepared and returned page proof. Final editing and proofreading were done almost exclusively by senior editors, although they occasionally requested help from junior staff during the process. Once the page proof was returned to the printer, it was too late to fix errors. Happily they were few, especially considering the huge number of entries in each volume, not to mention the fact that collective indexes inevitably were being prepared simultaneously—often with different rules for naming compounds.

A Few Representative People

A look at names on the *Chemical Abstracts* masthead during the early and mid-1960s suggests considerable ethnic diversity. A few thumbnail sketches illustrate the diversity and cosmopolitan nature of the staff at that time and are meant to provide a feel for the ambience and collegiality we enjoyed.

Mary Magill headed the Organic Index Editing Department. She had earned a Ph.D. in chemistry from

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Ohio State University many years earlier, at a time when it was unusual for a woman to be a scientist. She decided to pursue a career in chemistry while taking her first chemistry course in high school. In her sophomore year in college her professor took her to see a woman scientist, and they tried to talk her out of further study in chemistry because of the difficulties faced by women at that time. In spite of the daunting challenge of pursuing a male-dominated field, Mary went on to become a talented chemist, a fine editor, and a wonderful administrator. She was named "Outstanding Career Woman of 1963" by the Columbus, Ohio, *Citizen-Journal* (Tabor, 1964).

John Stone was Mary's assistant and a formula indexer *par excellence;* moreover, he was a character. He resided at the YMCA, drove a vintage Oldsmobile car, and virtually lived at CAS. Because of his seniority and dedication, he was allowed to keep plants, a black-and-white TV, and a hot plate in his office—his home away from home. Everyone knew that John made a lot of money, but everyone wondered what he did with it. Just as we were planning our move to the current CAS campus with its new buildings, John bought an airplane. Shortly thereafter, he began taking flying lessons. During groundbreaking ceremonies he flew over those of us attending, waved his wings, and seemed to lose control for a highly memorable moment.

Norman Donaldson, an organic index editor, was an Englishman who started his family before moving to this country and becoming a naturalized American. Norman loved to tell stories and, when asked about his children's nationality, he announced cheerfully that they were "half and half." One half was given a British inflection, while the other was plainly American.

Konrad Kossman, an organic indexer, was a German—another naturalized American citizen, but one who had fought on the German side during World War II. His children, while watching the then-popular TV show *Combat,* asked him if he was "one of those 'Krauts.'" He sighed and said, "Yes, I was one of those 'Krauts.'" Like his former foe Donaldson, he enjoyed telling stories.

Kurt Loening headed the Nomenclature Department. Had he lived earlier, he might have been "one of those Krauts" during World War I but certainly not World War II. Kurt was unwilling to speak about his childhood and adolescence in Nazi Germany, even with his family, saying he "couldn't remember" (Loening, 2000). This was hard to believe from a man who was able to recall not only the names of obscure chemical compounds but also the names of people he had met decades before. I think his position was essentially the antithesis of "never forget or forgive" and involved a feeling of obligation not to pass along hatred or blame to children for the transgressions of earlier generations.

It is impossible to give credit to everyone I remember. However, I want to mention Val Metanomski, who was known as an excellent general editor at *Chemical Abstracts* long before he became internationally known for his work in polymer nomenclature. And in addition I want to thank James E. Rush who had arrived at CAS six weeks before me and was therefore an authority. He showed me the ropes and became a lifelong friend and a diligent coauthor.

Asians and African Americans were in evidence on both the professional and the clerical staff. Although this is no longer considered remarkable, it was noteworthy in the early 1960s and had nothing to do with affirmative action. People were hired on the basis of their ability to do the work.

Nomenclature and Vocabulary Control

All of us were responsible for nomenclature, and the naming and indexing of chemical compounds was our bible (Chemical Abstracts Service, 1962). However, Kurt Loening was preeminent as head of the Nomenclature Department. Along with Leonard Capell and Donald Walker, he really specialized in naming compounds. Vocabulary control was, and remains, essential for printed indexes. If there is no such control—that is, if synonyms and homographs are allowed to proliferate—there will be enormous scattering of information throughout an index. While this may seem quaint to generations accustomed to computer-based systems permitting instant access to virtually everything, it was a major concern at the time.

Capell retired before we moved to the new campus, and Walker remained as a principal consultant on compounds with ring structure. As mentioned earlier, Casimir Gladys eventually assumed these tasks, having specialized in steroids before that. Loening, however, was uniquely responsible for resolving disputes between indexers and editors on how compounds were to be named for both annual and collective indexes. These disputes were never rancorous but involved committee meetings between department heads and the indexers and editors with expertise in the areas concerned. Other things being equal, the names chosen conformed to precedents. That is, if the names had appeared in earlier indexes, they were chosen again unless they had been voted against

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at the outset of a new collective index period. Each new collective period was viewed as an opportunity to review the suitability of names. Younger staff tended to prefer systematic names; older staff held out for traditional common ("trivial") nomenclature.

One thing I noticed immediately was that the senior staff often invoked "the user"—that is, the person who would be reading the index—in their arguments for employing traditional names. I once had the bad grace to ask if CAS had ever done a user survey and received nothing but scowls in reply. Social science was not exactly in vogue.

The absence of surveys aside, the evidence then and now supports the elders' advice. Readers of popular trade magazines like *Chemical and Engineering News* could care less about preferred index names. Preferred index names may not be those to which readers are accustomed. Figure 3 provides an example that may make the point. Any chemist would be able to recognize the first name in the caption and to visualize the structure of the compound. Moreover, the roots of the name are deeply embedded in the history of chemistry. Although it may not be obvious to the nonchemist, phthalimide is a cyclic, nitrogen-containing derivative of phthalic acid, and the etymology of its name goes back to naphtha(lene). One will find such names routinely in *Chemical and Engineering News* and similar publications and probably always will. Nevertheless, authorities at *Chemical Abstracts* later (during the 1970s) decided that such names should go by the wayside for the Ninth Collective Index. What was the replacement for this particular compound's name? They chose the second entry in the caption: 2-phenyl-1*H*-isoindole-1,3(2*H*)-dione. While this is a perfectly legitimate name for such a heterocyclic compound, it seems almost perverse to a practicing chemist. What happened to the old admonition of indexing compounds where the user would expect to find them?

The answer is simply that the controversy was becoming increasingly irrelevant. The era of database searching with user-friendly software had begun, not only with the advent of the Registry System but also with other developments that eventually would permit searchers to use whatever names they preferred.

Another Word about Computers

Changes in computer hardware during the early 1960s have already been mentioned, but there were simultaneous developments in software. The cold war, the launch of *Sputnik* in 1957, and other world events resulted in nearly frantic efforts to try using computers

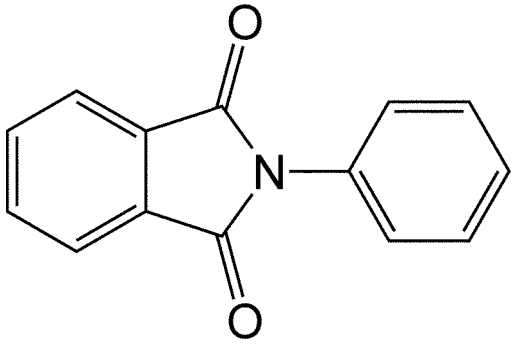

Figure 3. *Phthalimide, N-phenyl-, or 1*H*-isoindole-1,3(2*H*)-dione, 2-phenyl-.*

for what at that time were unrealistic things, especially natural language translation. While limitations of both hardware and software doomed these undertakings, that did not stop the massive infusion of funds for research and development. Nor was the money entirely wasted. Although translation efforts failed, interesting new software and programming languages were developed, including COMIT, SLIP, LISP, IPL-V, SNOBOL, and eventually PL/I and others (Sammet, 1969). Regardless of their individual merits, all of them incorporated ancient innovations leading to procedures that are now commonplace, the most obvious of which is word processing.

In the early 1960s some of us thought these techniques offered an opportunity to treat chemical nomenclature as a subset of natural language. Since mostly nouns were involved, it should have been easy to write programs to convert one name into another. In fact, one could do this, especially with the newer third-generation computers and improved software, but it was still cumbersome and expensive compared with dealing with Dyson's or Wiswesser's compact linear notations. Systematic names had the advantage of being linear notation that chemists could read and pronounce, but they were often too long and required too much storage space and processing speed for the necessary transformations (Garfield, 1962; Davis, 1967, 1969).

Moreover, there was the enormous success of the Registry System. What ultimately mattered was the structure of a compound. Once that was uniquely determined, one could attach whatever names one wanted, along with physical properties and pertinent bibliographic information.

A Word about Words

Chemists, like other scientists, are dependent on technology, and they sometimes become enamored of major

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developments such as the digital computer. In the process they may forget other things of fundamental importance, one of which is language. There is "romance" in certain names, and examples in the literature of chemistry are numerous. The origin of *phthalimide* has been mentioned above. However, there are many others. Some say, for example, that nepetelactone, the active ingredient of catnip, is named for the Italian town Nepete. That may be true, but close examination of the etymology suggests that the town's name and that of the compound probably come from a Latin rendering of the Etruscan word for *catnip*. We may never know for sure. In any case it is now possible, thanks in part to the pioneering work of computational linguists and innovative software designers in the 1950s and 1960s, to generate structures and formulas from a great variety of names, not just preferred index terms (see "Additional Links and References" in Davis, 2001).

Conclusion

We have been released from the labor-intensive, tedious manual indexing procedures required nearly a half century ago. In addition, thanks to the technological innovations begun during that era, we now have the best of two worlds: the ability to store and retrieve chemical information based on structural data, and the ability to search for and generate chemical compound names—not just rigidly systematic index terms but also those that any practicing chemist might use and prefer.

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