Coverage of Inorganic Heterocycles in *Chemical Abstracts*†

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This paper reports the results of two parallel searches for references on inorganic heterocycles by using the *Chemical Abstracts* (CA) Index of Ring Systems and an issue-by-issue search of weekly CA issues. Since several classes of inorganic ring systems are not covered by the CA Index of Ring Systems, only a partial overlap between the two searches is achieved. The distribution of references among the CA sections is discussed critically. While the CA *Index of Ring Systems* is highly useful in the retrieval of inorganic rings, some improvements in the coverage can still be made. The separation of a subsection on inorganic ring systems within CA Section 78 is suggested.

INTRODUCTION

Inorganic heterocycles have been known for a long time, but only in the last 20 years has this branch of modern chemistry emerged as a self-consistent field.[1–6] For most of the time, inorganic heterocycles were investigated within the chemistry of individual elements, mostly nonmetals, and several monographs illustrate this approach.[7–9] This tendency is also reflected in the indexing of inorganic ring compounds in abstracting journals and other secondary literature. Thus, the terms "inorganic ring systems" or "inorganic heterocycles" seldom appear in indexes. Only individual rings are usually indexed, and an integrated view, regarding the study of these compounds as an independent discipline, is usually absent. For this reason, it is very difficult, if not nearly impossible, to keep track of the main general developments and tendencies of the field as a whole. An attempt at a computer retrieval of the literature dealing with inorganic heterocycles, based on a profile search under this subject, would lead to meager results. The only way is to know in advance which inorganic rings are known and to search for each individual ring. This can be done by computer, provided the nomenclature used is known for each type of ring.

This paper reports the results of an experiment carried out with the aim of finding all the papers dealing with inorganic ring systems, covered by Vol. 92 (1980) of *Chemical Abstracts* (CA). The conclusions reached are in agreement with previous observations, related to the coverage in other CA volumes, and therefore the analysis of a single volume is rather illustrative.

To define the scope of this search, it must be emphasized that *only carbon-free ring systems were considered.* This delimitation was interpreted broadly to include mono- and polycyclic systems containing nonmetals and non-transition-metal rings. Rings containing transition metals were also included, but their retrieval implies some difficulties. Of course, the presence of organic groups as substituents on an inorganic (carbon free) ring did not prevent inclusion of such compounds in our search.

SEARCHING PROCEDURE

The search of ring systems in a given volume of *Chemical Abstracts* can be carried out with the aid of the Index of Ring Systems, published at the end of each semiannual CA Formula Index. The Index of Ring Systems lists all organic (carbon containing) and inorganic (carbon free) rings, including both mono- and polycyclic systems. The information provided by this index includes the ring formula (composition) and ring name. The later is very important, since there is no unique system of naming inorganic rings, and even *Chemical Abstracts* uses various procedures for naming different types of inorganic homo- and heterocycles.[10] When the name of each ring is known, the next step is to search the CA Chemical Substance Index. The information thus obtained includes the list of derivatives of each ring (with some other properties, reactions, etc.) and the list of abstracts (abstract numbers) of all references dealing with a ring. With the aid of these abstract numbers, the full references can be readily identified in the weekly issue of *Chemical Abstracts*, manually or with the aid of a computer (if computer tapes are available). The procedure followed is illustrated in Figure 1, and the list of references thus obtained will be called here List Number One.

A parallel (manual) search was carried out by consulting each weekly issue CA Sections 29 (Organometallic and Organometalloidal Compounds), 75 (Crystallization and Crystal Structure), and 78 (Inorganic Chemicals and Reactions). These sections are the most likely to contain the references dealing with inorganic ring systems. The list of references thus obtained will be called here List Number Two.

COMPARISON OF THE INDEX-BASED SEARCH WITH THE ISSUE-BY-ISSUE SEARCH

The two lists, obtained as described above, cannot be identical, because the issue-by-issue search covered only three CA sections. Even if an issue-by-issue search would cover all sections (which is practically impossible as it would be an extremely tedious and time-consuming job), the two lists would not be identical, for the reasons discussed below. A comparison of the results obtained in the two searches is shown in Figure 2.

In our search of CA Vol. 92 (1980), List Number One contained 217 references, of which 65 references came from CA Sections 29, 75, and 78. All these 65 references were also found in List Number Two, which contained a total of 193 references. Thus, the issue-by-issue search is at least as efficient as the index search, since all the references covered in the three overlaping sections were retrieved both by the index and the issue-by-issue search. Moreover, the issue-by-issue search produced another six references from the three sections, which were not retrieved through the index search, although the rings mentioned in these references are covered by the Index of Ring Systems. This may be a cause of alarm, since it reveals some gaps in the indexing procedure.

A total of 122 references, in List Number Two, dealing with carbon-free ring systems, not covered in the Index of Ring Systems, were retrieved only in the issue-by-issue search and could not be identified through the ring index search. This fact deserves some comments.

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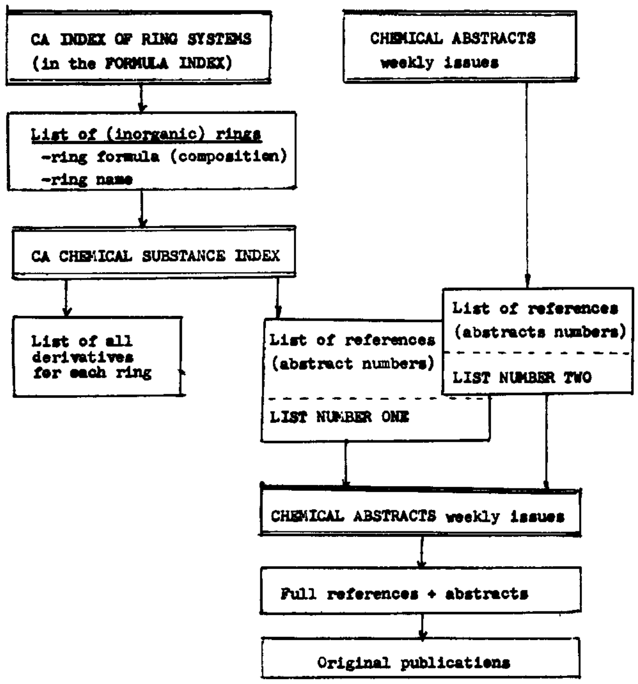


Figure 1. Steps of a literature search on inorganic ring systems (two parallel procedures).

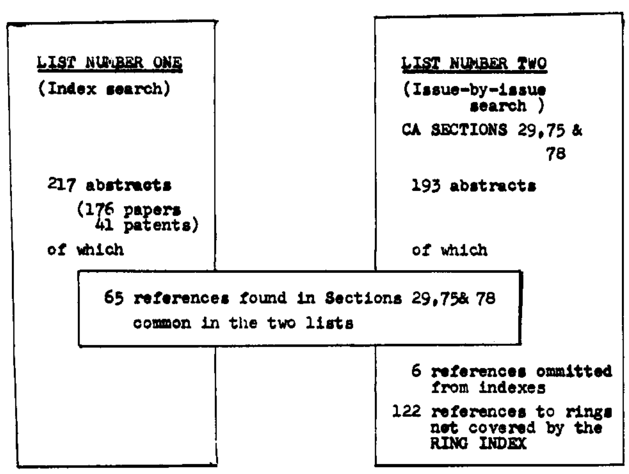


Figure 2. Comparison of results obtained in two parallel searches.

References not covered by the Index of Ring Systems include the following types of compound.

(a) Cyclic borates, phosphates, silicates, germanates, metaphosphimates [e.g., abstracts no. **92**:68043w (bicyclic borate $[B_4O_5(OH)_5]^{2-}$), **92**:50416k (cyclotetrasilicate $Si_4O_{12}^{8-}$), **92**:103435z (cyclotetraphosphate or tetrametaphosphate $P_4O_{12}^{4-}$), **92**:189505g (cyclic germanate $Ge_3O_9^{3-}$), 157016g (trimetaphosphimate $O_6P_3N_3H_3^{3-}$)]. To find these rings one has to consult the CA Chemical Substance Index under the appropriate entries, *in addition* to the CA Index of Ring Systems.

(b) Cyclic sulfur allotropes and their oxides (e.g., S_6 and S_7, abstract no. 87254g; S_6O, abstract no. 189496e).

(c) The three-membered P_3 ring as a ligand in transition-metal complexes, e.g., (triphos)Co(μ-η^3-P_3)$Cr_2(CO)_{10}$ (abstract no. **92**:94554h).

(d) Inorganic (carbon free) chelate rings of various types containing transition metals (e.g., the pyrazolylborato, pyrrazolylgallato, pyrrazolylphosphine, diphosphinoamine, and polyphosphine chelates shown in Figure 3 with their abstract numbers).

(e) Other inorganic rings containing transition metals (metallocycles) such as those illustrated in Figure 4.

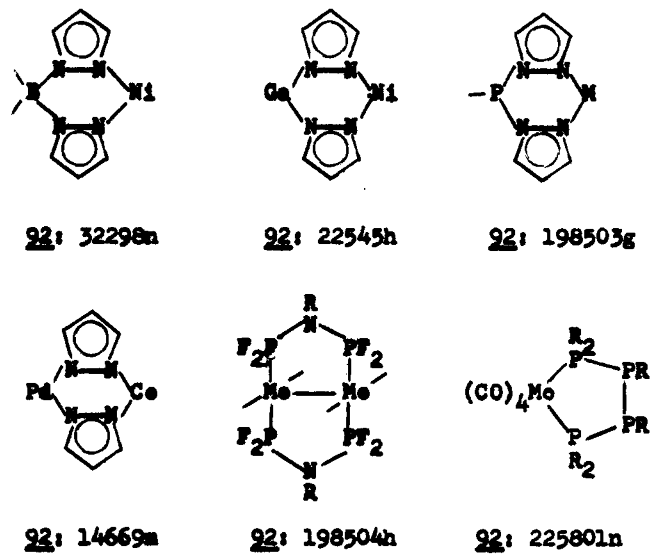


Figure 3. Inorganic (carbon free) chelate rings not covered by the Index of Ring Systems [the numbers are those of CA Vol. 92 (1980) abstracts in which these rings are cited].

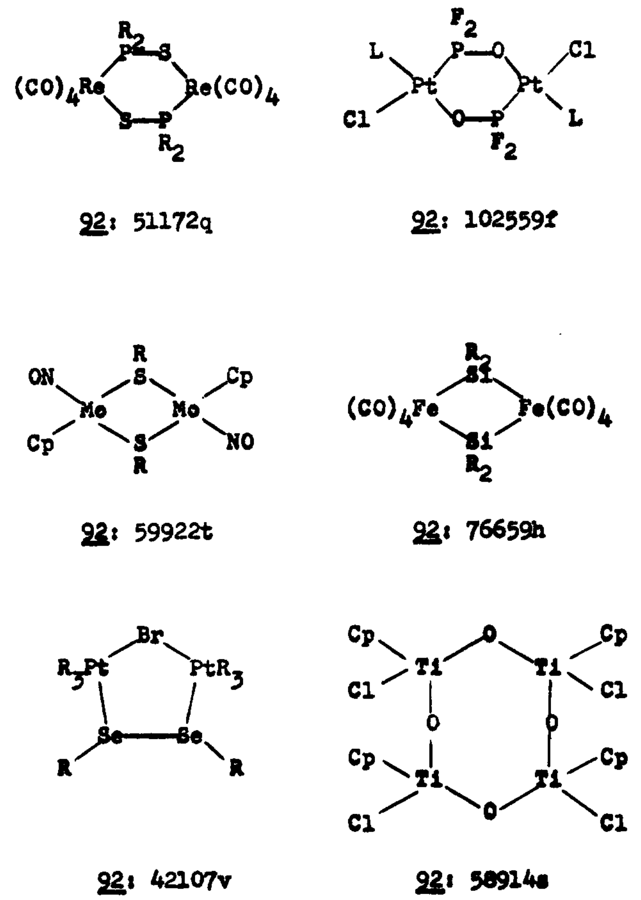


Figure 4. Some other inorganic metallocycles not covered by the Index of Ring Systems.

The issue-by-issue search also revealed some accidental omissions from the CA Chemical Substance Index and the Index of Ring Systems. Thus, the following abstracts were not retrieved through these indexes: (a) references dealing with sulfur–nitrogen rings, e.g., **92**:208164 ($Cl_3S_3N_3$) and **92**:173777m $[(S_7I)_2I]^+$; (b) references dealing with cubane-type polycyclic structures, e.g., **92**:197401k (P_4N_4 cubane), **92**:198450n (Sn_4N_4 cubane), and **92**:224644a (Cu_4Cl_4 cubane); (c) various others, e.g., **92**:215491w (Si_3P_3, Si_2P_4, and SiP_3 rings), **92**:172811f ($Me_8Ph_2Si_6O_7$ bicyclic siloxane), and **92**:164024m (spirotitanadisilazane). In all these cases only

Table I. Distribution of Abstracts in CA Sections

section no.	section title	no. of abstracts
29	Organometallic and Organometalloidal Compounds	41
22	Physical Organic Chemistry	30
35	Synthetic High Polymers	27
36	Plastics Manufacture	18
78	Inorganic Chemicals and Reactions	17
38	Elastomers	10
28	Heterocycles	9
73	Spectra	9
75	Crystallization and Crystal Structure	7
49	Industrial Inorganic Chemicals	6
25	Noncondensed Aromatic Compounds	4
27	Heterocyclic Compounds	4
39	Textiles	4
65	General Physical Chemistry	4
23	Aliphatic Compounds	3
63	Pharmaceuticals	3
68	Phase Equilibriums, Chemical Equilibriums, Solutions	3
1	Pharmacodynamics	2
4	Toxicology	2
37	Plastics Fabrication and Uses	2
42	Coatings, Inks and Related Products	2
76	Electric Phenomena	2
3	Biochemical Interactions	1
5	Agrochemicals	1
51	Fossil Fuels, Derivatives and Related Products	1
54	Extractive Metallurgy	1
62	Essential Oils and Cosmetics	1
66	Surface Chemistry and Colloids	1
79	Inorganic Analytical Chemistry	1
80	Organic Analytical Chemistry	1
total papers abstracted in CA Vol. 92 (1980)		217

the issue-by-issue search provided the references cited.

Some references found by issue-by-issue search (in List Number Two), e.g., no. **92**:5793v, **92**:172857a, and **92**:208209g, dealing with the cyclic compound S_4N_4, are listed in the CA Chemical Substance Index under the entry "nitrogen sulfide N_4S_4". The Index of Ring Systems does ot indicate this entry under eight-membered rings for the ring composition N_4S_4. If seems to be general that known cyclic compounds like cyclic sulfur allotropes, metaphosphates, and sulfur–nitrogen molecules or ions are not indexed under the appropriate systematic names in the CA Chemical Substance Index if the cyclic structure is not mentioned in the primary publication. Such references can be found only by an additional search of the CA Formula Index or under their trivial names in the CA Chemical Substance Index.

DISTRIBUTION OF REFERENCES AMONG CA SECTIONS. POSITIVE AND NEGATIVE ASPECTS

The distribution of the 217 references in List Number One, retrieved with the aid of the index searching, among the various CA Sections is shown in Table I.

The largest number of references are cited in CA Section 29 (Organometallic and Organometalloidal Compounds). This is due to the fact that in most cases inorganic ring compounds are prepared as organo-substituted derivatives. The unexpectedly large number of references found in CA Section 22 (Physical Organic Chemistry) is caused by the (unjustified) treatment of organo-substituted derivatives of inorganic rings as organic compounds. Such references were sometimes included in CA Section 22 even when the organic substituted played a minor role and the properties were determined by the inorganic ring skeleton. The content of the references included in CA Section 22 is illustrated in Table II and deals mostly with spectral properties of inorganic ring derivatives. In this respect it is surprising that CA Section 73 (Spectra) contained a relatively small number of references related to the same topics. This distribution will certainly be altered with CA Vol. 96 (1982) when some changes in the organization of CA subject sections will be introduced.[11] Thus, CA Section 29 (Organometallic and Organometalloidal Compounds) will expand its content to include organic derivatives of oxo acids of boron and group 5A elements even if they contain no carbon–metal bond (formerly in CA Sections 23–28), physical organic studies and structure determinations of these compounds (formerly in CA Section 22), and metal heterocyclic compounds containing no carbon atom in the ring (formerly in CA Sections 23–28).[11] Therefore the CA Section 29 will become the most likely place to find inorganic ring systems when they bear organic substituents.

Table II. Distribution of References in CA Sections 22, 73, and 65. Selected Examples

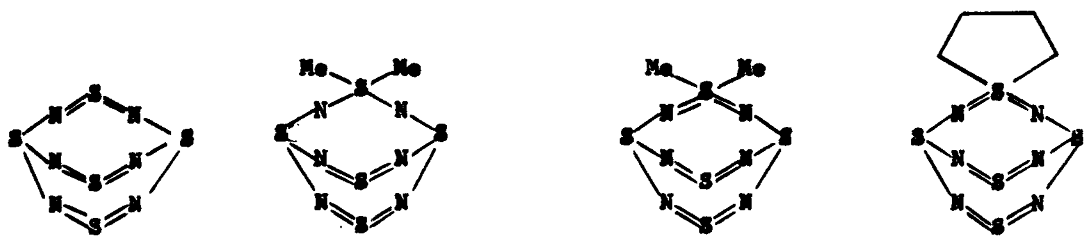
CA section	subject	rings	examples (abstract no.)
22 (Physical Organic Chemistry)	vibration spectra	P_5, P_6	**92**:5710r
	mass spectra	Si_3O_3	**92**:5719a
	NMR spectra	Si_5, Si_6	**92**:5963a
	UV spectra	SiN, SiO	**92**:21652d
	basicity	Si_3N_3	**92**:57980y
	free radicals	B_3N_3	**92**:21736j
		P_3N_3	**92**:21776x
73 (Spectra)	NMR spectra	N_3Sn_3	**92**:31545k
		O_4Si_4	**92**:32414d
		N_3P_3	**92**:101881t
		N_2P_2	**92**:31517c
	vibration spectra	N_3P_3	**92**:13113p
65 (General Physical Chemistry)	OM calculations	B_3N_3	**92**:28872j
		N_5	**92**:65008c

Table III. References Dealing with the Use of Inorganic Ring Derivatives in Polymer Synthesis

CA section	subject	examples (abstract no.)
35 (Synthetic High Polymers)	polymerizable cyclosiloxanes	**92**: 6982t, 6998c, 7173s, 23001q, 23076t, 42438d, 42439c, 59426w, etc.
	polymerization of cyclophosphazenes	**92**: 7088t, 22872n, 59430t, 59456f
36 (Plastics Manufacture and Processing)	polymerization of cyclosiloxanes	**92**: 7240m, 59554m
	boroxine derivatives as curing agents for epoxy resins	**92**: 7324s
	polymerization of cyclophosphazenes	**92**: 59516a, 59679f, etc.
37 (Plastics Fabrication and Uses)	polymerization of cyclosiloxanes	**92**: 111892m, 216482f
38 (Elastomers)	cyclosiloxanes	**92**: 24001b, 24025m, 77811x, 95445k, 130356f, 130358h
	cyclosilazanes	**92**: 130303n, 182359d
	cyclophosphazenes	**92**: 130362e

The large number of references found in CA Sections 35 (Synthetic High Polymers), 36 (Plastics Manufacture), and 38 (Elastomers) is related to the use of some inorganic ring derivatives, mostly cyclophosphazenes and organocyclosiloxanes, as starting materials for the synthesis of inorganic chain polymers, as illustrated in Table III.

The inclusion of some references in CA Sections 27 (Heterocyclic Compounds—One Heteroatom) and 28 (Heterocyclic Compounds—More than One Heteroatom) deserves comment. The inclusion of papers dealing with the use of P_2S_2 inorganic ring derivatives $(RPS_2)_2$ as reagents in the synthesis of organic heterocyclic compounds (e.g., abstracts no. **92**:41863b,



92: 93838s CA Section 23 (Aliphatic compounds)

92: 94476j CA Section 29 (Organometallic

92: 94165g CA Section 27 (Heterocycles)

Figure 5. *Chemical Abstracts* citation of three closely related references.

92:58652e, **92**:110754f, **92**:215352b, **92**:215368m) is justified. However, the inclusion of references dealing with $S_5N_6(CH_2)_4$ (abstract no. **92**:94165g), $(ClSN)_3$ (abstract no. **92**:128623x), and S_4N_2 derivatives (abstract no. **92**:41896q) and of abstracts no. **92**:128863a, **92**:198327c, and **92**:198430f (dealing with PN rings) shows a strong bias in favor of organic chemistry. In these references the inorganic ring is treated *as an organic heterocycle* (containing only heteroatoms), or a carbon-containing heterocyclic part of a complex molecule present on a main inorganic ring skeleton determines the placement of the abstract. This organic chemistry bias is also reflected in including reactions of $(Cl_2PN)_3$ with epoxides (abstract no. **92**:58217s) and of $(ClSN)_3$ with $N(SnMe_3)_3$ (abstract no. **92**:93838s) in CA Section 23 (Aliphatic Compounds) or of P_2N_2 ring formation from PCl_3 and aniline (abstract no. **92**:146357t), preparation of an *N*-phenyl derivative of the S_7N ring (abstract no. **92**:76032g), and reaction of $(ClSN)_3$ with Ph_2CNLi (abstract no. **92**:12956g) in CA Section 25 (Noncondensed Aromatics). In all these cases, it is obvious from the content of the references cited that their main point of interest is the inorganic ring, while the organic aspect is only marginal.

Many references, mostly dealing with uses, biological activity, or some specific properties of inorganic cyclic derivatives, are listed in appropriate CA sections, as shown in Table I. This is completely justified from the viewpoint of the applied chemistry practitioner, but cross-references at the end of Sections 78 or 29 would be highly desirable.

The fact that the study of the chemistry of inorganic heterocycles has not yet gained recognition and acceptance as a self-contained discipline is mirrored in the lack of a consistent well-defined policy in covering inorganic hetero- and homocycles in *Chemical Abstracts*. This is already obvious from the discussion presented above but is beautifully illustrated by the example given in Figure 5. This shows three papers dealing with closely related compounds, all derived from the same bicyclic skeleton, S_5N_6, covered in three different CA Sections. Thus, papers reporting the synthesis of S_5N_6 compounds with a cage structure (abstract no. **92**:93838s),[12] the molecular structure of the S_5N_6 dimethyl derivative (abstract no. **92**:94476j),[13] and the preparation of a spiro derivative of S_5N_6 (abstract no. **92**:94165g)[14] are cited in different places in a way which again reflects a strong organic chemistry bias. None of these abstracts appears in Section 78 (Inorganic Chemicals and Reactions); even the first paper, reporting the purely inorganic compound S_5N_6, is included in Section 23, because of the presence of a dimethyl derivative in the same paper.

CONCLUSIONS AND FINAL COMMENTS

The analysis of the *Chemical Abstracts* practice in the coverage of inorganic ring systems (homo- and heterocycles) reveals that the retrieval of references dealing with such compounds is not a straightforward job. The main features can be summarized as follows.

(a) The inclusion of inorganic rings in the CA Index of Ring Systems is of great use in the retrieval of all carbon-free rings (and their derivatives) containing nonmetals and nontransition metals. Without this tool it would be almost impossible to search for inorganic homo- and heterocycles in the CA Chemical Substance Indexes, as long as no unique nomenclature is used.

(b) The practice of classifying the abstracts according to the use, investigation technique (e.g., spectroscopy), or other properties of the compounds described in individual papers is acceptable, if adequate cross-referencing between CA sections is provided.

(c) Criticism can be addressed to *Chemical Abstracts* in relation to the strong bias in favor of organic chemistry demonstrated by (1) classification of individual derivatives according to the organic substituents rather than the parent ring system and (2) inclusion of some inorganic rings as "heterocycles with more than one heteroatom" (in CA Section 28).

(d) The lack of coverage of inorganic rings containing transition metals and some nonmetal rings in the CA Index of Ring Systems and accidental omissions of some references in the indexes suggest possible future improvements in the preparation of these useful tools.

On the basis of the facts discussed in this paper, I suggest that the Chemical Abstracts Service should adopt a well-defined policy in covering inorganic ring systems, including the adoption of a unified system of nomenclature and the awareness and recognition by editors and document analysts (abstractors) of inorganic heterocycles as a self-consistent discipline. The separation of a subsection entitled "Inorganic Ring Systems" within CA Section 78 (Inorganic Chemicals and Reactions), with adequate cross-referencing to other sections, would also be of great help to *Chemical Abstracts* users. An excellent example is the cross-referencing provided now by CA Section 75 (Crystallization and Crystal Structure). The separation of inorganic (carbon free) ring derivatives within CA Section 29 would also be highly desirable. All these could help in establishing a new *CA Selects* series dealing with inorganic ring systems.

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A Pharmaceutical Information Manager's Viewpoint on R & D Information Resource Management†

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The long time span required for product development and the multidisciplinary nature of research, combined with regulatory constraints, pose unusual problems in information resource management (IRM) in pharmaceutical research and development. Management styles, personnel selection criteria, automated systems, and information content are discussed. Service evaluation is highly subjective and dependent on a satisfied user.

INTRODUCTION

Two decades ago, new regulatory requirements were put in place by U.S. Food and Drug Administration in the pharmaceutical industry. Much has been written in recent times about "drug lag", the need for patent life extension, and the impact of tight regulations on innovation. It is important to note the types of changes that have occurred because these impact the information management activities. Laubach[1] has quoted figures which are significant. Thus, the increased time for development (2-9 years from 1962 to 1976) and the increased cost ($4-$54 million over the same time) are indicative of the complexities under which both proprietary and published data/information must be collected, evaluated, and disseminated.

Along with the regulatory constraints, other changes have occurred. The hurdles over which new product candidates must pass are now higher because the easy problems have been solved, enhanced safety requirements are in vogue, and new diagnostic/detection capabilities have been discovered. Life is more complex in spite of the enhanced sophistication in methodology.

The development of a new human drug may involve the collaborative efforts of representatives from 30-50 distinct scientific disciplines—bringing a greatly increased scope to the need for data/information requirements.

In summary then, our backdrop involves a multidisciplinary requirement for collecting, indexing, storing, retrieving, evaluating, and disseminating data/information/knowledge over a decade of time between project definition and market introduction. Both proprietary and published information are required from manual and computer-based systems.

PHILOSOPHY FOR IRM

Different management styles bring different degrees of emphasis, as well as a different set of "buzz" words. If we interpret management as the ability to accomplish results through the efforts of others, then several functions/activities are needed, viz., planning, organizing, leading, and controlling. A brief word about these is in order.

Planning needs to be at a number of levels. Most important is the strategic (longer range) type. Here, the environment—technical, organizational and political—needs to be assessed. The mission of the organization, a translation of that mission into perceived information requirements, and a notion of the information-gathering habits of the user population are all important. Some insight into the perceived value of information to management, as well as how (by what means) the transfer should occur, must be determined. For example, one philosophy says, "stock a room with books and journals and let those who wish come to use". Another says a more proactive stance should prevail; i.e., the information ought to be "packaged" to meet individual or small group needs and then be sent to the desks of those requiring it. The latter is obviously more expensive but may also be more effective in dealing with the "flood" of information. Planning under the first philosophy would be quite different than under the latter.

Organization may likewise be based on a number of premises. My personal preference is for a mission-oriented or functional organizational scheme. Thus, though many units distinguish between published and proprietary information, the user frequently needs both and should not have to satisfy his/her needs by going to separate units. It is true that security requirements are different for the two types of data, but the utility for problem-solving or decision support may be equal. Widely separated geographic units do require extra site supervision, but failure to recognize the functional similarities at several sites leads to duplication of resources.

Leading in an information resource management operation must be concerned with subordinates and with clients. A major problem which all staff managers face is the question of authority. As for clients, we must recognize that we are *long* on responsibility and *short* on authority. Hence, our goal must be to do our homework, espouse useful technology, and be sure

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