Structure Versus Reality in Polymer Nomenclature*

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The rationale behind structure-based nomenclature is discussed for organic polymers for which structural information is known or can be assumed. Such nomenclature is contrasted with traditional polymer nomenclature based on source. Also considered are problems of naming polymeric materials for which little structural information is available or which are inherently irregular in structure. For these, codes are preferred to linguistic nomenclature wherever possible. A code for members of the "ABS Resin" family is suggested.

Nomenclature development involves research in linguistics. As with most research, there are basic and applied aspects. There are those who generate new and sometimes forbidding systems of nomenclature, i.e., language, designed to accommodate the problems of the future. And there are those who must apply that language now to the problems of today. On the one hand, some seem to forget that humans, as well as machines, must speak our language; on the other hand, some of our practical men seem loath to leave the language of yesterday. The purpose of this paper is to meld these positions and views in the field of polymer nomenclature and to show that a step toward the unfamiliar need not mean a departure from chemical reality.

We can define nomenclature either in terms of systems of classification or as a system of naming the members of a given classification. While there may be many classifications, it is sensible to keep the number of naming systems at a minimum, and certainly there should never be more than one system for each class. Unfortunately, this ideal is rarely met in science. In chemistry, for example, the classification called "Organic compounds" enjoys no fewer than five recognized systems of nomenclature at the present time. One of these, substitutive nomenclature, has obvious advantages, and one is hopeful that in the near future those five will become one. This is not to say that any one system must serve any or all related classifications: however desirable, a single system is not absolutely necessary for both inorganic and organic compounds, for example. As the relationship between classifications becomes more diffuse, nomenclature systems need not be compatible at all—the nomenclature of distillation units has no requirement of compatibility with the nomenclature of the substances being distilled.

Organic polymers, as chemical substances, are evidently members of the class of organic compounds. Substitutive nomenclature in organic chemistry has as its rationale the chemical structure of the compounds being named. It is reasonable to extend such nomenclature to organic polymers and this has been done. However, when organic polymers are subdivided on the basis of structural knowledge, it is realized that the number of polymers whose structure is truly known is small indeed. We have polymers whose structures are (a) known, (b) partially known, (c) assumed, and (d) unknown. For (a), (b), and (c), a structure-based nomenclature compatible with that for organic compounds is not only desirable, it is necessary. For subclass (d), such a nomenclature is not only unnecessary, it is impossible. This is reality. The substance being named is for practical purposes a formulation for which most ingredients and some properties, but not the structure, are known. It might be an "acrylic resin having such-and-such viscosity." If this description is sufficient, so be it, but under no circumstances should structure be invoked and an attempt made to name the unnameable on this basis.

STRUCTURAL REALITY IN ORGANIC COMPOUNDS AND POLYMERS

In advocating a common structural basis for naming both "small" and "polymeric" substances, we must consider the contents of the bottle of material to which we are attempting to attach a rational label. If we accept structure as a basis for labeling a container of organic molecules, are we not ignoring some of the realities of chemistry? No matter what we call the contents, there will be more than one kind of molecule present. Such molecules might be isomers or outright impurities. The steric structure of most of the molecules may be incompletely known. Even though we know most of the history of the substance, we still find structure, to the extent it is known, a more useful basis for the label.

For polymers in subclasses (a), (b), and (c), a very similar situation exists. While a bottle of a given polymeric substance may contain mostly molecules whose main chains are chemically and structurally similar, those chains always have a number of different lengths. The ends of the chains may be chemically quite unlike the chains themselves, and the chains in turn may have structural or chemical defects and impurities at random points. The history of the substance may be very well known, but it is of little service in describing the substance to be named.

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Clearly, there is much in common between small organic compounds and their polymeric brothers as far as structural reality is concerned; with the same parents, they might be expected to have similar surnames. In both instances, one affixes a label on the basis of the main kind of molecule in the bottle, and the impurities and imperfections, the isomers and chain branches and end groups, can be ignored unless there is a specific reason for including them in the label. In the latter case, no harm is done to a structure-based name by adding a few descriptors: "2,4-Pentadiene Containing 38% *cis*-Isomer" and "Poly(ethylene) Containing 1% Double Bonds" are perfectly good labels.

TRADITION IN POLYMER NOMENCLATURE

Polymers have usually been named on the basis of their history or their source, real or imagined. When there were only a few polymers to be named, the names themselves were of little importance other than that each material needed a unique name. Since little was known of the structure of the material itself, it was reasonable to name a polymer as simply a multiple of the compound from which it was made. Poly(styrene) is the polymer made from styrene and poly(ethylene) is the polymer made from ethylene, and never mind what the structure is as far as description is concerned. When the polymer was made from two components by a condensation process, a name based on both sources seemed cumbersome, and a hypothetical source was used. Names such as poly(ethylene terephthalate) resulted. All that is required to visualize "ethylene terphthalate" as a source material is an imaginary ring-opening reaction.

The tradition of naming polymers on the basis of source or process is strongly embedded in polymer chemistry. So strong is this tradition that the few polymers that have been named on some other basis, such as structure, are as often as not related to a source or process by that ever-present imagination. Poly(methylene), for example, is often thought of as "the polymer made from diazomethane," even though the name is structure-based.

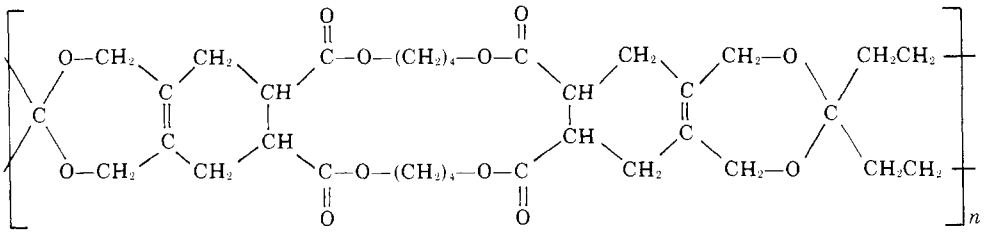
In recent years, it has become increasingly evident that the traditional source-based polymer nomenclature is inadequate to the task of providing unique names for most polymers. There are too many instances where a single monomer could, depending on the polymerization process, yield more than one polymer. Acrolein, for example, might polymerize by way of either the aldehyde or the vinyl group. The polymer called "poly(oxyethylene)" on a structure basis might conceivably be made from a number of different monomers, and therefore could be given the same number of source-based names. These are simple examples. For existing polymers such as a source-based name is not only inadequate, it is nonsense. This is the reality that traditional polymer nomenclature must face. Polymers such as the last example can be named on a structural basis—poly[(6,6a,7,9,10,11,12,14a,-15,16,21,21a,22,24,25,26,27,29,29a,30-eicosahydro-7,14,22,29-tetraoxo-1H,5H,14H,20H-[1,6,11,16]-tetraoxacycloeicosino-[3,4-h:13,14-h′]bis[2,4]benzodioxepin-3,18-diylidene)-18,-18-diethylene]—and although the name itself may be rather cumbersome, the polymer will be uniquely described in terms understandable to chemists familiar with organic nomenclature. Polymer science can no longer afford its traditional nomenclature. The price to be paid for a complete change to systematic structure-based nomenclature is that of converting from one simple name to another simple name for common polymers—poly(styrene) becomes poly(phenylethylene) and a dividend is gained, since the latter name is more readily accommodated by the computer.

NOMENCLATURE OF POLYMERS OF UNKNOWN STRUCTURE

The polymers of subclass (d), noted earlier, present the real problems of polymer nomenclature. These are the materials for which almost no structural information is available. Even the "history" may be murky or the source unknown, as for certain natural polymers. Polymers for which the source is known but for which any inferred structure is irregular also fall into this category. These would include the so-called random copolymers and the "compositions of matter" often seen in the patent literature. No attempt should be made to develop or apply a structure-based nomenclature system to such materials.

This is not to say that labels for these substances must be devoid of rationality. Trivial names for this purpose are usually irrational—they are simply nouns designating a thing or group of things, like rubber or concrete. Trade or ex-trade names like nylon fall into the same class. Sometimes these names are modified in some way to convey information, as in nylon-6/6. Usually, such modification conveys less information than is desired, possibly because of the mixed rationality-irrationality of the names.

There is no single or easy answer to the problem of rational names for members of vaguely defined families of polymers. For certain kinds of materials, however, a partial solution may be found in the use of codes rather than names. This is not a new approach, and it has in fact been utilized successfully in describing members of one class of rather complex macromolecules—the proteins. For an example of how a code might be devised, take the so-called "ABS resins." This family name, itself a code, covers a multitude of polymeric products derived from acrylonitrile (A), butadiene (B), and styrene (S).



Specific polymers of regular structure obtained from these monomers can be named by a structure-based nomenclature system, but most of these products are known only from the processes by which they were made and by an analysis of their compositions. Thus, a code name based on percentage composition might be "A(30)B(50)-S(20) Resin." Additional descriptors can be used to give process details. For example,

S(20)-A(30)-g-polyB[A(10)B(70)S(20)]

would represent the grafting of a mixture of 20 parts of styrene and 30 parts of acrylonitrile to poly(butadiene) to give an ABS Resin, 70% of which was derived from butadiene, 10% from acrylonitrile, and 20% from styrene. A mixture of two polymers might be labeled "Poly[A(30)-S(20)]-mix-polyB(70)." Such codes are simply a matter of establishing and learning a group of conventions. They are a form of shorthand and as such are more convenient than the paragraph of description that may be required for an individual family member. These codes are useful but they are in no sense nomenclature, and they will never replace language.

SUMMARY

Our language can handle the real world of organic polymers on a rational structural basis if polymer chemists are willing to make the same assumptions they have long accepted as organic chemists. This will allow the kind of flexibility needed for both today and the distant tomorrow, including the requirements of both chemist and computer. Such acceptance also forces the polymer chemist to break with some traditional language habits with which he is very much at home.

At the same time, it must be recognized that no rational language system can handle the irrational. Polymers having irregular structures must be labeled on the basis of information available. The label may be either a modified trivial name, which communicates little, or it can be an artificial code. In the latter case, word confusion is reduced, and if simple and transmittable terms are used, communication can indeed take place.

A New Notation System for Indexing Polymers*†

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A new linear notation system, based on carbon, its bonding, and the number of hydrogens attached to it, is evaluated as an indexing mechanism for polymers from the viewpoint of the structural repeating unit for linear polymers and reactants for highly cross-linked polymers or resins. The system yields computer printouts in which structural classes, such as allyl, vinyl, and vinylidene, and amide, urethane, and ester polymers, are grouped together.

Polymer nomenclature problems caused by the increase in number and complexity of polymers make effective communication difficult.[1] As serious as these nomenclature problems are in the communication aspects, they are considerably more intractable in the indexing aspects. In response to these problems, we have considered the feasibility of the various notation systems described in the literature[2-6] for a possible solution.

Although most of the notation systems described yielded unambiguous and unique designations, each required major modifications for computer processing into a reasonably ordered arrangement. In summary, we found the established notation systems to be discordant with the needs of polymer chemists for bringing like things together and to be incompatible with computer processing.

Recently a new notation system was introduced which is based on carbon, carbon bonding, and hydrogens.[7,8] This notation system yields specific and unambiguous designations with the additional advantage of being in harmony with computer processing into chemically related arrangements. The application of this system to polymer structural indexing via computer is illustrated in this paper.

BASIS FOR POLYMER INDEXING

Polymers can be indexed on the basis of the monomers from which they are formed or on the basis of the actual structure of the repeating unit. We have chosen to use the structural repeating unit for all linear polymers: first, because it avoids ambiguities of one monomer forming more than one polymer or of more than one monomer forming the same polymer; and, second, to assure like polymer structures being grouped together. This is in agreement with the structure-based polymer nomenclature system presented in a report by the Nomenclature Committee of the Division of Polymer Chemistry of the American Chemical Society[1] and with the convincing arguments

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