scientist. After examination and acceptance by the Inorganic Chemistry Division, the proposal follows the accepted IUPAC procedure and is then submitted to the IUPAC Council for approval.

www.iupac.org/publications/pac/2002/7405/7405x0787.html

“Heavy Metals”—A Meaningless Term? (IUPAC Technical Report)

by J. H. Duffus
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 793-807 (2002)

Over the past two decades, the term “heavy metals” has been widely used. It is often used as a group name for metals and semimetals (metalloids) that have been associated with contamination and potential toxicity or ecotoxicity. At the same time, legal regulations often specify a list of “heavy metals” to which they apply. Such lists differ from one set of regulations to another and the term is sometimes used without even specifying which “heavy metals” are covered. However, there is no authoritative definition to be found in the relevant literature. There is a tendency, unsupported by the facts, to assume that all so-called “heavy metals” and their compounds have highly toxic or ecotoxic properties. This has no basis in chemical or toxicological data. Thus, the term “heavy metals” is both meaningless and misleading. Even the term “metal” is commonly misused in both toxicological literature and in legislation to mean the pure metal and all the chemical species in which it may exist. This usage implies that the pure metal and all its compounds have the same physiochemical, biological, and toxicological properties, which is untrue. In order to avoid the use of the term “heavy metal,” a new classification based on the periodic table is needed. Such a classification should reflect our understanding of the chemical basis of toxicity and allow toxic effects to be predicted.

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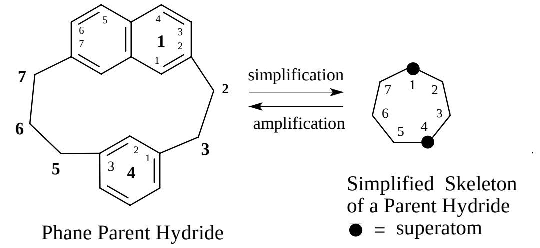
Phane Nomenclature. Part II. Modification of the Degree of Hydrogenation and Substitution Derivatives of Phane Parent Hydrides (IUPAC Recommendations 2002)

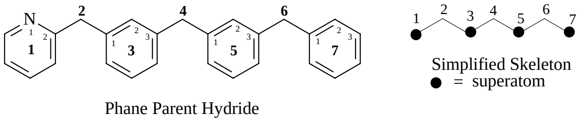
by H. A. Favre, D. Hellwinkel, W. H. Powell, H. A. Smith, Jr., and S. S.-C. Tsay
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 809-834 (2002)

Phane nomenclature is a new method for building names for organic structures by assembling names that describe component parts of a complex structure. It is based on the idea that a relatively simple skeleton for a parent hydride structure can be modified by an operation called “amplification,” a process that replaces one or more special atoms (superatoms) of the simplified skeleton by multiatomic structure(s).

Examples:



Simplified skeletal name: cycloheptaphane
Phane parent hydride name:
1(2,7)-naphthalena-4(1,3)-benzenacycloheptaphane



Simplified skeletal name: heptaphane
Phane parent hydride name:
1(2)-pyridina-3,5(1,3),7(1)-tribenzenaheptaphane

The multiatomic structure is a fully saturated or mancude ring or ring system. A mancude ring or ring system contains the maximum number of noncumulative double bonds. In the amplification operation, each superatom is replaced by an amplificant denoted by an “amplification prefix” attached to a stem called a “simplified skeletal name.” The latter ends with the term “phane” and is formed according to the principles for deriving names of saturated hydrocarbons. Accordingly, all of the atoms implied by the skeletal name, except for those replaced by amplification prefixes are, by convention, saturated carbon atoms. An amplification prefix is derived from the name of the corresponding cyclic parent hydride by the addition of the terminal letter “a” with elision of a terminal vowel of the parent hydride name, if present. Phane prefixes thus resemble the prefixes, such as “oxa,” “aza,” etc., that indicate replacement of a single atom, usually a carbon atom, by a different atom.

The locants in front of the parentheses in the phane parent hydride name identify the positions of the superatoms in the simplified skeleton that are replaced by the ring structure specified by the amplification prefix immediately following. By the same token, they also identify the positions of the rings and ring systems in the phane parent hydride. These locants are determined by the inherent numbering of the simplified skeleton and the seniority of the rings and ring systems in the phane parent hydride. The locants within the parentheses specify the atoms of the ring structure specified by the amplification prefixes that are linked to the adjacent normal atoms of the simplified parent skeleton.

In addition to the basic principles, rules and conventions of Phane Nomenclature, Part I [*Pure Appl. Chem.* 70(8), 1513-1545 (1998)] contains the fundamental methodology for numbering phane parent hydrides and the application of skeletal replacement (“a”) nomenclature for naming heterophane parent hydrides.

Part II of Phane Nomenclature describes derivatives of phane systems formed by substitutive nomenclature. The following nomenclatural features are described: indicated and added hydrogen, order of seniority for numbering, substituents expressed as suffixes, substituents cited as prefixes, phane parent hydrides modified by addition or subtraction of hydrogen atoms, and polyfunctional derivatives.

www.iupac.org/publications/pac/2002/7405/
7405x0809.html

Harmonized Guidelines for Single-Laboratory Validation of Methods of Analysis (IUPAC Technical Report)

by M. Thompson, S. L. R. Ellison, and R.Wood
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 835-855 (2002)

Method validation is one of the measures universally recognized as a necessary part of a comprehensive system of quality assurance in analytical chemistry. In the past, ISO, IUPAC, and AOAC International have cooperated to produce agreed protocols or guidelines on the “design, conduct and interpretation of method performance studies,” on the “Proficiency testing of (chemical) analytical laboratories,” on “internal quality control in analytical chemistry laboratories,” and on “the use of recovery information in analytical measurement.” The Working Group that produced these protocols/guidelines has now been mandated by IUPAC to prepare guidelines on the single-laboratory validation of methods of analysis. These guidelines provide minimum recommendations on procedures that should be employed to ensure adequate validation of analytical methods. A draft of the guidelines has been discussed at an International Symposium on the Harmonization of Quality Assurance Systems in Chemical Laboratory, the proceedings from which have been published by the UK Royal Society of Chemistry.

www.iupac.org/publications/pac/2002/7405/
7405x0835.html

Polyaniline. Preparation of a Conducting Polymer (IUPAC Technical Report)

by J. Stejskal and R. G. Gilbert
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 857-867 (2002)

Eight persons from five institutions in different countries carried out polymerizations of aniline following the same preparation protocol. In a “standard” procedure, aniline hydrochloride was oxidized with ammonium peroxydisulfate in aqueous medium at ambient temperature. The yield of polyaniline was higher than 90% in all cases. The electrical conductivity of polyaniline hydrochloride thus prepared was 4.4 ± 1.7 S cm^{-1} (average of 59 samples), measured at room temperature. A product with defined electrical properties could be obtained in various laboratories by following the same synthetic procedure. The influence of reduced reaction temperature and increased acidity of the polymerization medium on polyaniline conductivity were also addressed. The conductivity changes occurring during the storage of polyaniline were monitored. The density of polyaniline hydrochloride was 1.329 g cm^{-3}. The average conductivity of corresponding polyaniline bases was 1.4×10^{8} S cm^{-1}, the density being 1.245 g cm^{-1}. Additional changes in the conductivity take place during storage. Aging is more pronounced in powders than in compressed samples. As far as aging effects are concerned, their assessment is relative. The observed reduction in the conductivity by ~10% after more than one-year storage is large but, compared with the low conductivity of corresponding polyaniline (PANI) base, such a change is negligible. For most applications, an acceptable level of conductivity may be maintained throughout the expected lifetime.

www.iupac.org/publications/pac/2002/7405/
7405x0869.html

Studies on Biodegradable Poly[hexano-6-lactone] Fibers. Part 3. Enzymatic Degradation in Vitro (IUPAC Technical Report)

by T. Hayashi, K. Nakayama, M. Mochizuki, and T. Masuda
Pure and Applied Chemistry, Vol. 74, No. 5, pp. 869-880 (2002)

This report describes how poly(hexano-6-lactone) (PCL) fibers were enzymatically degraded by a hydrolase in vitro. The extent of degradation of PCL fibers was examined by weight loss, mechanical properties loss such as tensile strength and ultimate elongation decreases, and visual observations by scanning electron