IUPAC Projects

SCOPE/IUPAC International Symposium on Endocrine Active Substances

The Scientific Committee on Problems of the Environment (SCOPE) and IUPAC are jointly organizing an International Project on "Environmental Implications of Endocrine Active Substances: Present State of the Art and Future Research Needs." The project started in April 2000 and is scheduled to be completed in March 2003. The SCOPE/IUPAC International Symposium on Endocrine Active Substances, to be held 17-21 November 2002 in Yokohama, Japan, will constitute a major milestone for the project. All of the project contributors (ca. 60 experts) will present papers dealing with the following topics:

- Molecular Mode of Action of Nuclear Receptors; Fundamentals for Understanding the Action of Endocrine Active Substances
- Environmental Fate and Metabolism of Endocrine Active Substances
- Effects of Endocrine Active Chemicals in Rodents and Humans, and Risk Assessments for Humans
- Effects of Endocrine Active Substances in Wildlife Species

In addition, six supplementary workshops will be held:

- Effectiveness of QSAR for prescreening of endocrine disruptor hazard
- Toxicogenomics as a rational approach to endocrine disruptor research
- The need for establishing integrated monitoring programs
- Simple, rapid assay for conventional definitive testings of endocrine disruptor hazard
- Precautionary principle/approach and weight of evidence in endocrine disruptor issues
- Risk management options for endocrine disruptors in national and international programs

See the symposium announcement in *CI*, Vol. 23, No. 5, p. 156, September 2001.

http://www.iupac.org/projects/2000/2000-016-1-600.html

Highlights from Pure and Applied Chemistry

Presenting recently published IUPAC technical reports and recommendations

Generic Source-Based Nomenclature for Polymers (IUPAC Recommendations 2001)

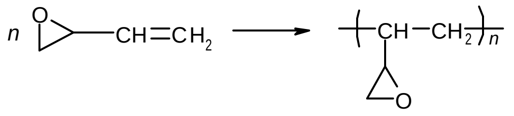
by E. Maréchal and E. S. Wilks
Pure and Applied Chemistry, Vol. 73, No. 9, pp. 1511-1519 (2001).

Present-day high-performance polymer materials are becoming increasingly difficult to name concisely with existing macromolecular nomenclature. Simple and practical names that refer to the monomer source (i.e., source-based nomenclature) are therefore highly desirable; thus, the rules that lead to such names need to be spelled out. That task was undertaken by an international group of experts of the former IUPAC Commission on Macromolecular Nomenclature. Their recent recommendations on generic source-based nomenclature for polymers describe an unambiguous naming system that is as rigorous as, but more practical than, structure-based nomenclature. This generic naming system complements the earlier source-based method, which in some cases leads to ambiguous names.

A generic source-based name comprises two parts:

1. polymer class (generic) name followed by a colon;
2. the actual or hypothetical monomer name(s) (source), always parenthesized in the case of a copolymer. (See figure for an example.)

In this document, five rules are presented and illustrated by 20 examples; the formula, the structure-based name, the source-based name, and the generic source-based name of the polymer are given for each example.



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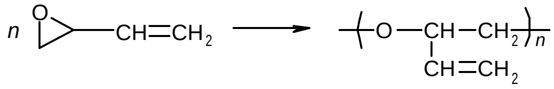

II

Structure-based names:
I. poly(1-oxiranylethylene)
II. poly[(oxy(1-vinylethylene)]

Source-based name:
I and II have the same source-based name: poly(vinyloxirane).

Generic source-based names
I. polyalkylene:vinyloxirane
II. polyether:vinyloxirane

In some cases, only generic source-based nomenclature gives unambiguous names, for example, when a polymer has more than one name or when it is obtained through a series of intermediate structures. The rules concern mostly polymers with one or more types of functional groups or heterocyclic systems in the main chain, but to some extent they are applicable also to polymers with side-groups, carbon-chain polymers such as vinyl or diene polymers, spiro and cyclic polymers, and networks.

http://www.iupac.org/publications/pac/2001/7309/7309x1511.html

Quantum Chemical B3LYP/cc-pvqz Computation of Ground-State Structures and Properties of Small Molecules with Atoms of $Z \leq 18$ (Hydrogen to Argon) (IUPAC Technical Report)

by Rudolf Janoschek
Pure and Applied Chemistry, Vol. 73, No. 9, pp. 1521-1553 (2001).

Since density functional theory achieved a remarkable breakthrough in computational chemistry, the important general question "How reliable are quantum chemical calculations for spectroscopic properties?" should be answered anew. In this project, the most successful density functionals, namely the Becke B3LYP functionals, and the correlation-consistent polarized valence quadruple zeta basis sets (cc-pvqz) are applied to small molecules. In particular, the complete set of experimentally known diatomic molecules formed by the atoms H to Ar (there are 214 systems) is uniformly calculated, and calculated spectroscopic properties are compared with experimental ones.

Computationally demanding molecules, such as open-shell systems, anions, or noble gas compounds, are included in this study. Investigated spectroscopic properties include spectroscopic ground state, equilibrium internuclear distance, harmonic vibrational wavenumber, anharmonicity, vibrational absolute absorption intensity, electric dipole moment, ionization energy, and dissociation energy. The same computational method has also been applied to the ground-state geometries of 56 polyatomic molecules up to the size of benzene. Special sections are dedicated to nuclear magnetic resonance chemical shifts and isotropic hyperfine coupling constants. Each set of systems for a chosen property is statistically analyzed, and the above important question "How reliable . . . ?" is mathematically answered by the mean absolute deviation between calculated and experimental data, as well as by the worst agreement. In addition to presentation of numerous quantum chemically calculated spectroscopic properties, a corresponding updated list of references for experimentally determined properties is presented.

http://www.iupac.org/publications/pac/2001/7309/7309x1521.html

Standards in Isothermal Microcalorimetry (IUPAC Technical Report)

by Ingemar Wadsö and Robert N. Goldberg
Pure and Applied Chemistry, Vol. 73, No. 10, pp. 1625-1639 (2001).

Isothermal microcalorimetric techniques have been much improved during the past decades, and several types of instruments are commercially available. Application areas include, for example, ligand binding studies, dissolution and sorption measurements, estimation of the stability of chemical substances and technical products, and measurements of metabolic reactions in living cellular systems.

Most isothermal microcalorimeters are calibrated by the release of heat in an electrical heater positioned in the calorimetric vessel or in its close proximity. However, in some cases it is difficult to conduct electrical calibration experiments, which will closely mimic the heat flow pattern of the process or reaction under investigation. This can lead to a significant error in the calibration value and, in some cases, the use of some