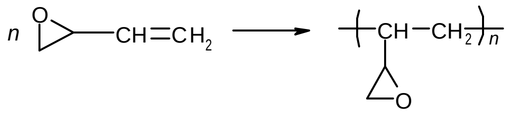
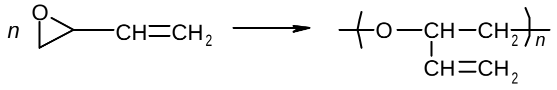


I



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 chemical calibration would therefore be preferable. Regardless of which calibration technique is used, it is often desirable to quantitatively control the overall performance of an instrument by use of a suitable test reaction. Simple and reliable test reactions are also very suitable for the training of experimenters. In order to allow a close comparison between results from chemical calibrations or test experiments and results from a calorimetric investigation, it is important to have many different chemical calibration and test reactions available.

In this report, guidelines are presented on the use of standardized chemical test and calibration reactions suitable for use in different areas of isothermal microcalorimetry. The focus is on reactions suitable for use under ambient conditions. Further, a standardized terminology in describing the characteristics of isothermal microcalorimeters is proposed. “Nanocalorimeters,” usually indicating calorimeters with a detection limit approaching the nanowatt range, are in this report not distinguished from “microcalorimeters.”

The Task Group responsible for the project was: I. Wadsö (Chairman), A. E. Beezer, R. N. Goldberg, G. Olofsson, K. Murphy, J. Rouquerol and J. Sipowska.

http://www.iupac.org/publications/
pac/2001/7310/7310x1625.html

Critical Evaluation of Stability Constants of Phosphonic Acids (IUPAC Technical Report)

by Konstantin Popov, Hannu Rönkkömäki,
and Lauri H. J. Lajunen
Pure and Applied Chemistry, Vol. 73, No. 10, pp. 1641-1677 (2001).

Organophosphonate chelating compounds are widely used in a broad variety of applications.Their ability to prevent precipitation of calcium salts at substoichiometric concentrations (threshold effect) finds wide application in water treatment for scale inhibition. Phosphonates, particularly EDTPH and DTPPH, are used extensively in laundry detergents. These materials are also used as corrosion inhibitors, in industrial cleaning and in peroxy bleach stabilization. Uses of organophosphonates span applications in flame-resistant polymers, photographic processing, ore flotation (aminophosphonic surfactants), actinide separation processes, and analytical chemistry. Recently, organophosphonates have been identified as promising reagents for the creation of so-called “structurally tailored” materials and microporous materials, in catalysis, and in the electrochemical treatment of polluted soils.

The high biological activity of carboxyalkylphosphonates, aminoalkylphosphonates, and alkylenediphosphonates makes them useful agents as components of microfertilizers and pesticides in agriculture, as well as drugs and diagnostic reagents in biology and medicine. Annual industrial output of organophosphonates is in the thousands of tons.

The broad and intensive applications of organophosphonates require reliable data on the stability constants of the corresponding complexes in order to permit equilibrium modeling and prediction of the important technological, environmental, and pharmacokinetic equilibria. As phosphonates resist biodegradation, chemical speciation calculations based on numerical equilibrium data are of extreme importance for applications such as environmental science, waste management, agriculture, scale inhibition, magnetic resonance imaging, behavior of radiopharmaceuticals in blood plasma, and many others.

The data of interest are partly accumulated in some monographs, reviews, and compilations of stability constants. Recently, two computer databases have become commercially available. The IUPAC Stability Constants Database (SC-Database) is the more comprehensive. For organophosphonates, some data in the “critically evaluated compilations” are not consistent with later, more precise results. These are therefore rejected in the present work.

This study critically evaluated available experimental data on stability constants of proton and metal complexes for 10 phosphonic acids [methylphosphonic acid, 1-hydroxyethane-1,1-diylbisphosphonic acid, dichloromethylenebisphosphonic acid, amino-methanephosphonic acid, *N*-(phosphonomethyl)glycine, imino-*N*, *N*-bis(methylenephosphonic acid), *N*-methylamino-*N*, *N*-bis(methylenephosphonic acid), nitrilotris(methylenephosphonic acid), 1,2-diaminoethane-*N*,*N*,*N*´,*N*´-tetrakis-(methylenephosphonic acid), and diethylenetriamine-*N*,*N*,*N*´,*N*´´,*N*´´-pentakis-(methylenephosphonic acid)]. For the latter phosphonate, all the data are rejected, as well as protonation constants [HL]/[H][L] for three other ligands. Higher-quality data are selected and presented as “Recommended” and “Provisional.”

This review is generally based on the data published in the period 1965-1996, but some earlier and later publications are also included. The data collection embraced databases Chemical Abstracts, and the personal collections of the authors.

http://www.iupac.org/publications/
pac/2001/7310/7310x1641.html