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Recommendations on Measurement and Analysis of Results Obtained on Biological Substances Using Isothermal Titration Calorimetry (IUPAC Technical Report)

Frederick P. Schwarz, Timm Reinisch, Hans-Jürgen Hinz, and Avadhesha Surolia

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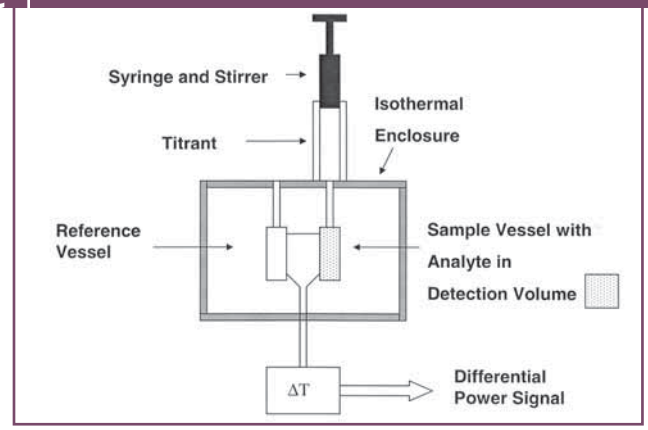

Basic ITC instrument, consisting of a sample vessel containing the analyte solution and a vessel containing a reference solution (e.g., buffer solution) within an isothermal enclosure.

Isothermal titration calorimetry (ITC) is widely used to determine the thermodynamics of biological interactions, including protein-protein, small molecule-protein, protein-DNA, small molecule-DNA, and antigen–antibody interactions. An ITC measurement consists of monitoring the transfer of heat between an analyte solution in a sample vessel and a reference solution in a reference vessel upon injection of a small aliquot of titrant solution into the sample vessel at a fixed ITC operating temperature. A binding isotherm is generated from the heat-transferred-per-injection data. Values for the binding constants, the apparent binding enthalpies, and the apparent ratio of the amount of titrant to analyte for the binding reaction are then determined from fits of a binding model (whether it is a single site, identical multi-site, or an interacting multi-site binding model) to the binding isotherm.

Prior to the fitting procedure, corrections should be made for contributions from extraneous heat of mixing determined separately from injections of the titrant into just the dialysate/buffer solution. Ultra-high binding constants, which cannot be directly determined from an ITC measurement, can be determined by a displacement ITC method where injections of the tight-binding titrant into a solution of a weaker-binding titrant-analyte complex displaces the weaker-binding titrant from the complex. The Michaelis and catalytic constants can be determined for an enzyme reaction from injections of a substrate or enzyme titrant into an enzyme or substrate analyte solution. This article suggests several binding reactions to use to check the operating performance of the ITC. The reporting of ITC results must be specific with regard to the composition of the titrant and the analyte solutions, the temperature, and the model used in the analysis.

www.iupac.org/publications/pac/80/9/2025/

Nomenclature for Rotaxanes and Pseudorotaxanes (IUPAC Recommendations 2008)

Andrey Yerin, Edward S. Wilks, Gerard P. Moss, and Akira Harada

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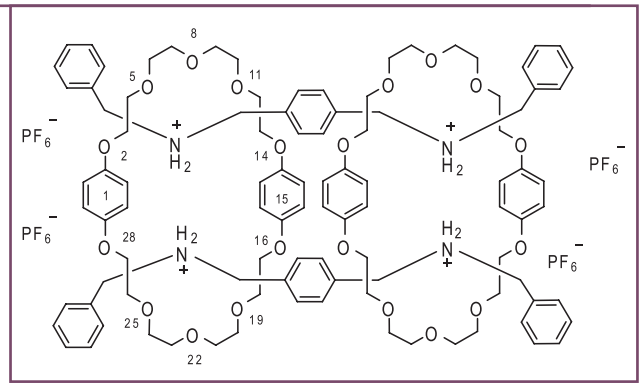

A Type 2.2 [4]pseudorotaxane with symmetrical components: **[4]{[2][1,1′-(1,4-phenylene)bis(*N*-benzylmethanaminium)]-rotaxa-[2][2,5,8,11,14,16,19,22,25,28-decaoxa-1,15(1,4)dibenzenacyclooctacosaphane]} tetrakis (hexafluoridophosphate).**

Rotaxanes were first represented pictorially in 1958 as in situ intermediates in the synthesis of [2]catenanes. Rotaxanes were proposed as a new type of species (though not referred to as pseudorotaxanes or rotaxanes) in 1961, and shown to exist in 1967. However, it was not until 1971 that Schill introduced a nomen-

clature system for rotaxanes. In 2000, Vögtle and coworkers proposed a generic nomenclature system in which Schill's description was extended to include information about mechanical or covalent linkages within the components of the rotaxane to distinguish between intermolecular and intramolecular rotaxanes. Nevertheless, the proposed nomenclature cannot unambiguously describe the whole range of rotaxane structures reported in the literature.

This article specifies a systematic nomenclature for rotaxanes that includes the description of structure, composition, and isomerism of rotaxanes. This article discusses only rotaxanes in which none of the components is macromolecular, but the naming principles specified also can be used to name macromolecular rotaxanes. Specific recommendations for naming rotaxanes with at least one polymeric component will be published in a separate document.

Because the structures of rotaxanes are often large, in most cases throughout this article schematic presentations of rotaxanes and their components are used. Full chemical structures of rotaxanes and their systematic names are given.

www.iupac.org/publications/pac/80/9/2041

Solubility Data Series

SDS Volume 83: Acetonitrile: Ternary and Quaternary Systems

V.P. Sazonov, et. al.

J. Phys. Chem. Ref. Data, 2007, Vol. 36, No. 3
pp. 733–1131; doi: 10.1063/1.2539811

The mutual solubility and liquid-liquid equilibria of acetonitrile ternary and quaternary systems with liquid solvents are reviewed in this article. The solvents include water, inorganic compounds, and a variety of organic compounds such as hydrocarbons, halogenated hydrocarbons, alcohols, acids, esters, and nitrogen compounds. A total of 191 ternary and 35 quaternary systems whose properties were described in the chemical literature through 2000 are compiled. For 37 systems sufficient data were available to allow critical evaluation. All data are expressed as mass % and mole fractions as well as the originally reported units. Similar reviews of gas, liquid, and solid solubilities for other systems were published earlier in the Solubility Data Series.

SDS Volume 84: Solubility of Inorganic Actinide Compounds

Jiri Hála and H. Miyamoto

J. Phys. Chem. Ref. Data, 2007, Vol. 36, No. 4
pp. 1417-1736; doi: 10.1063/1.2741386

This volume presents the solubility of inorganic compounds of actinides except for carbonates, which are included in Volume 74 of this series, and nitrates, which are covered in Volume 55. Also included are solubility data of compounds such as organosulfates, phosphates, and arsenates, which are not covered in Volume 74. The predominant part of this volume covers solubility data of thorium, uranium, neptunium, and plutonium compounds. Fewer data have been published for americium compounds and very few for compounds of actinium, protactinium, and transamericium elements. The literature has been covered up to the end of 2004. Documents that remained unavailable to the editor, and could not be included in the volume are listed in the appendix. For some compounds, it was not possible to show the Chemical Abstracts registry numbers since these have not been assigned.