

The Project Place

Solubility Data of Compounds Relevant to Human Health

Three of the priority subjects to be pursued by the Solubility Data Project over the next three years were announced in *CI*, Vol 24, No. 6, November 2002, p. 20-21. The following volumes—which belong to the fourth major field related to the solubility data of compounds relevant to human health—are to be published within the IUPAC-NIST Solubility Data Series.

Solubility of Substances Related to Urolithiasis

Improved solubility predictions for substances precipitating from complex body fluids would be of great benefit, given that, for instance, over one million Australians are currently suffering from kidney stones, causing the health system direct identifiable costs of over \$70 million a year. The prevention and treatment of crystal deposition in the human body are based on the understanding of the physico-chemical properties underlying the precipitation of the substances involved. Among these properties, the solubilities of the crystals are very important. In the scope of urolithiasis, there are more than 20 different types of kidney stones composed of calcium oxalate hydrates (mono-, di-, and trihydrate), ammonium magnesium phosphate (struvite), calcium phosphates (hydroxyapatite and brushite), uric acid and urates, cystine, and xanthine. Solubilities of these substances can be incorporated in databases of sophisticated software packages that permit solubility calculations in artificial urine solutions. The results of these simulations would lead to some understanding and/or useful suggestions regarding the cause, prevention, and treatment of renal or bladder calculi. In any case, proper modelling of the solubilities of these substances requires reliable solubility constants. Thus, it is necessary to critically assess the literature values reported for these substances. Recently, a review on this subject was published in *PAC*, Vol. 73, pp. 785-797 (2001).



www.iupac.org/projects/2002/2002-035-1-500.html

Solubility of Hydroxybenzoic Acids and Hydroxybenzoates

Hydroxybenzoic acids and related compounds are pharmaceutically important substances. In particular, 2-hydroxybenzoic acid has been widely used as a

medicine and a preservative for food products; 4-hydroxybenzoic acid alkyl esters have also been used as preservatives for food. The relation between the use of these substances and human health requires evaluation of the solubilities of 2-, 3-, and 4-monohydroxybenzoic acids and of 4-hydroxybenzoic acid alkyl esters in water, organic and mixed solvents. In this project, it is also intended to evaluate the solubilities of (a) 2- and 3-hydroxybenzoic acid in supercritical carbon dioxide containing organic solvents such as methanol and acetone, and (b) monohydroxybenzoates, 2,3-, 2,4-, 2,5-, 2,6-, 3,4- and 3,5- dihydroxybenzoic acid salts of alkali, transition, and rare earth metals in water and organic solvents.



www.iupac.org/projects/2002/2002-036-1-500.html

Solubility of Halogenated Aromatic Hydrocarbons

Halogenated derivatives of aromatic and polyaromatic hydrocarbons have been widely used as heat transfer fluids, organic diluents, plasticizers, fire retardants, pesticides, waxes, and more. However, recently it has been pointed out that some of these or their related compounds, of both synthetic and natural origin, can seriously interfere with reproductive function. From the pharmaceutical and environmental viewpoints, the solubilities of these substances are useful to elucidate the movement and persistence in the environment and to estimate the hazard or risk associated with them. Therefore, it is important to evaluate the solubilities of, for example, chlorinated benzenes, biphenyl, and dioxins in various media including single, binary, and/or multi-component solvents, micellar solutions, and polymer solutions.

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www.iupac.org/projects/2002/2002-037-1-500.html