Alcohols + Hydrocarbons + Water

Marian Góral et al
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IUPAC-NIST Solubility Data Series, Volume 101

This paper is Part 1 of a compilation and evaluation of the mutual solubilities of C_1 to C_{10} alcohols with hydrocarbons and water. This work incorporates compilations based on reports in the peer-reviewed scientific literature prior to the middle of 2012. The solubilities of ternary alcohol-hydrocarbon-water systems were reviewed in 1999 in Vol. 69 of the IUPAC Solubility Data Series.

Because the solubilities of alcohol-hydrocarbon-water systems are of considerable importance and widespread interest among several groups including industrial and environmental chemists, because the earlier volumes are now difficult to obtain and are over 19 years out of date (previous compilations were considered through 1992), and because a new technique of data evaluation has been developed, the decision was made to revise and update this work as a new volume.

This revised work will be published in three parts:

- Part 1: C_4–C_{10} Alcohols + Hydrocarbons + Water
- Part 2: C_1–C_3 Alcohols + Aliphatic Hydrocarbons + Water
- Part 3: C_1–C_3 Alcohols + Aromatic Hydrocarbons + Water

http://dx.doi.org/10.1063/1.4867621

ICTAC nomenclature of thermal analysis (IUPAC Recommendations 2014)

Trevor Lever et al.
Pure and Applied Chemistry, 2014
Volume 86, Issue 4, pp 545–553

The widespread use of thermal analysis by scientists as a laboratory technique carries with it a working vocabulary. This document is intended to provide those working in the field with a consistent set of definitions to permit clear and precise communication as well as understanding. Included in the document are the definitions of 13 techniques, 54 terms within the glossary, as well as symbols and units.

http://dx.doi.org/10.1515/pac-2012-0609

A database of water transitions from experiment and theory (IUPAC Technical Report)

Jonathan Tennyson, et al
Pure and Applied Chemistry, 2014
Volume 86, Issue 1, pp. 71–83

This technical report covers the outcome of an IUPAC task group formed in 2004 on “A Database of Water Transitions from Experiment and Theory” (project 2004-035-1-100). Energy levels and recommended labels involving exact and approximate quantum numbers for the main isotopologues of water in the gas phase, $H_2{}^{16}O$, $H_2{}^{18}O$, $H_2{}^{17}O$, $HD^{16}O$, $HD^{18}O$, $HD^{17}O$, $D_2{}^{16}O$, $D_2{}^{18}O$, and $D_2{}^{17}O$, are determined from measured transition frequencies. The transition frequencies and energy levels are validated using first-principles nuclear motion computations and the MARVEL (measured active rotational–vibrational energy levels) approach. The extensive data including lines and levels are required for analysis and synthesis of spectra, thermochemical applications, the construction of theoretical models, and the removal of spectral contamination by ubiquitous water lines. These datasets can also be used to assess where measurements are lacking for each isotopologue and to provide accurate frequencies for many yet-to-be measured transitions. The lack of high-quality frequency calibration standards in the near infrared is identified as an issue that has hindered the determination of high-accuracy energy levels at higher frequencies. The generation of spectra using the MARVEL energy levels combined with transition intensities computed using high accuracy ab initio dipole moment surfaces are discussed. The task group recommends further work to identify a single, suitable model to represent pressure- (and temperature-) dependent line profiles more accurately than Voigt profiles.

http://dx.doi.org/10.1515/pac-2014-5012

Definition of the transfer coefficient in electrochemistry (IUPAC Recommendations 2014)

Rolando Guidelli et al.
Pure and Applied Chemistry, 2014
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The transfer coefficient α is a quantity that is commonly employed in the kinetic investigation of elec-