

InChI 1.01

The IUPAC International Chemical Identifier, InChI version 1, was released in August 2006. The whole package, available at <www.iupac.org/inchi>, includes:

- InChI version 1 software version 1.01 documentation, and Windows and Linux (i386) executable programs
- InChI version 1.01 source code and Application Program Interface (API)
- InChI validation protocol
- What's new in InChI software version 1.01

This release includes the following new features:

- InChI validation protocol to establish whether software that includes the InChI algorithm produces valid InChI
- InChI reversal: InChI to structure conversion (connection table, bond orders, charges, stereochemical parities; the resultant structures have no coordinates; success rate on average is 99.7 percent)
- Several bug fixes that eliminate known InChI failures
- Several minor additional features

For more detail, see the Whats_New.pdf included in the package.

We express our gratitude to those who discovered and helped fix various problems with the software and validation protocol.

Q&A—Q: Why is the InChI version in this package 1, not 1.01?—**A:** The version of the chemical identifier (as

a string of characters derived from a chemical structure) is the same, only the software and documentation were updated. Therefore, the InChI version is still version 1.



See Tools of the Trade on page 12 for more information on InChI.

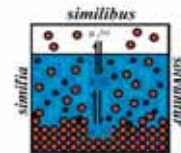
 www.iupac.org/projects/2004/2004-039-1-800.html

Dewen Zeng Receives the 2006 Franzosini Award

At the 5th Annual Meeting of the IUPAC Subcommittee on Solubility and Equilibrium Data, the Franzosini Award was presented to Dewen Zeng in appreciation of his scientific contributions to the Solubility Data Project.

Zeng received his Ph.D. in 2003 at TU Bergakademie Freiberg, Germany. During his Ph.D. project he worked under the supervision of Wolfgang Voigt (Institute of Inorganic Chemistry) on the thermodynamic modelling of salt-water systems. Zeng is a very active scientist who became an expert in thermodynamics and phase diagrams. After one year as a post-doc he returned to China and continued to work on modelling and evaluating solubilities and vapor pressures of salt-water systems.

At the 12th International Symposium on Solubility Phenomena, held in Freiberg, Germany, 24–28 July 2006, Zeng presented research conducted with Hongyan Zhou and Wolfgang Voigt on “Thermodynamic Consistency of Solubility and Vapour Pressure of a Binary Saturated Salt-Water System: II. $\text{CaCl}_2 + \text{H}_2\text{O}$.” See page 31 for a report on the symposium.



Dewen Zeng would like to contribute with his scientific experience to the activities of the solubility data group, particularly in respect to the oceanic salt project. Since Zeng is a native Chinese writer and speaker, he can provide access to Chinese literature on solubility phenomena, which is becoming more and more important to the solubility data group.

Zeng is a professor in the College of Chemistry and Chemical Engineering at Hunan University, Changsha, China.

 For more info about the Franzosini Award, its origin, and previous awardees, see <www.iupac.org/divisions/V/502/Franzosini-Award.html>.