INTERNATIONAL UNION OF
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InChI Software 1.03 Summary

In June 2010, IUPAC and the InChI Trust (www.inchi-trust.org) announced the release of version 1.03 of the software. This version integrates the generation of the standard InChI string and non-standard, customized strings as well as the corresponding InChIKeys. Options to generate the non-standard InChI within the same package as the standard InChI make it easier for organisations to use these additional options within their internal systems, conforming to their business rules. Version 1.03 also fixes a number of minor bugs. It clarifies how undefined/unknown stereochemistry is handled, and deals with some structure perception and stereo interpretation option issues.

The complete package contains the files listed below (each of them should be unpacked into a separate directory).

- INCHI-1-DOC.zip - contains documentation related to InChI/InChIKey identifiers v. 1 and InChI software v. 1.03 (2010).
- INCHI-1-BIN.zip - contains stand-alone executables for generating the InChI/InChIKey (Windows and Linux).
- INCHI-1-API.zip - contains code, VC++ projects and gcc makefiles of command-line program inchi-1, as well as of InChI generation library (plus sample applications which use the Library).
- INCHI-1-TEST.zip - contains the files representing various chemical and simple test suite for InChI/InChIKey software.

For the details, see 'RelNotes.pdf' document in INCHI-1-DOC and the 'readme.txt' files in the respective directories.

June 2010

Source Code Documentation *(March 2011)*

Documentation of the InChI source code, commissioned by the InChI Trust from Digital Chemistry Ltd, is now available for download from the InChI Trust website atwww.inchi-trust.org/index.php?q=node/14. It has been prepared with the aim of allowing developers who are maintaining, modifying or extending the code to understand the basis on which it was written, the principles underlying its organization and the main algorithms it implements. The document is not intended to reverse engineer the code, nor to provide a complete functional specification for InChI, but rather to provide an insight into how the code is constructed and what algorithms are used.

See Project Number: 2004-039-1-800

For a review of what is InChI and what it can be used for, see McNaught, A. “The IUPAC International Chemical Identifier: InChI - A New Standard for Molecular Informatics,” *Chemistry International*, Vol. 28, No. 6, p. 12, Nov-Dec 2006.