IUPAC INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

InChITRUST

InChI is..

IUPAC International Chemical Identifer (InChI)

- A unique identifier of a chemical structure serving as its digital signature
- A machine-readable string of characters derived solely from a structural representation of a chemical substance
- A project of IUPAC and the InChITrust

The purpose of InChI is...

- To streamline naming conventions for chemical compounds and reactions
- To uniquely identify a chemical substance, without ambiguity, providing a precise, robust, structure-derived tag for chemical substances
- To assist in merging and linking chemical databases

InChI is essential...

as the only structure representation standard in the public domain, open-source and freely available to the scientific community

The InChI Timeline

1999/2000
Steve Heller and Steve Stein initiate InChI project at the request of IUPAC

2005
Launch of InChI

2008
A fixed length (27 character) condensed digital representation of the InChI called the InChIKey was developed

2009
Formation of a Trust for a strategic vision and funding for the InChI project

2017
Latest version of InChI software was released along with InChI for reactions

And still more to come...

The InChI project is ongoing; not all of chemistry is yet covered by the software.

The vast majority of organic compounds can be encoded into InChIs, but many inorganic and organometallic compounds are still work in progress.

What do InChIs look like?

Chemical Compound	InChI	InChI-Key
Methanol	1S/CH4O/c1-2/h2H,1H3	OKKJLVBELUTLKV-UHFFFAOYSA-N
Lithium hydride	1S/Li.H	SIAPCJWMELPYOE-UHFFFAOYSA-N
Acetone	1S/C3H6O/c1-3(2)4/h1-2H3	CSCPPACGZOOCGX-UHFFFAOYSA-N

Make your own

The key component of InChI-enabled communication is a software package that encodes a chemical structure into a string of letters and numbers called an identifier.

The InChI software in action....

If both sender and receiver have the InChI software, they can:

Communicate chemical structures simply by encoding the structure into the string using the free software tool, transmit the unique identifier.

The receiver then decodes (with the identical software) the string back into a connection table.

The most current InChI software release can be downloaded from the InChI Trust download page (inchi-trust.org)

Be part of the InChI community...

Help build the chemical web and encourage others to do the same!

Explore more than **90 000 000** chemical compounds with an InChI here: pubchem.ncbi.nlm.nih.gov

Explore more than **156 000 000** chemical structures here: ebi.ac.uk/unichem

Join the discussion HERE

Learn more here

Videos by the InChI Trust:
inchi-trust.org

InChI Collection in J Cheminf:
biomedcentral.com/collections/InChI

Many InChIs and quite some feat
by Wendy A. Warr:
link.springer.com/article/10.1007%2Fs10822-015-9854-3
(or https://rdcu.be/M0kk)

Google tech:
youtube.com/watch?v=mpZj4b9eIYE

IUPAC page on InChI:
iupac.org/who-we-are/divisions/division-details/inch

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