

InChI: what is it and what will it be?

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The InChI is the **international chemical identifier**, providing dependable, canonical names for molecular structures.

The latest release, InChI v1.07, [1] has security enhancements and refactored code, building on v1.06. [1] The code is all available on GitHub. [1]

Work on the InChI continues

extended stereochemistry
tautomers
organometallics
molecular inorganics
polymers
nanomaterials
isotopologues
macromolecules
Applications are addressing new areas of InChI-based data-handling.
Mixture-InChI
Markush-InChI
Nano-InChI
Reaction InChI

The InChI is a very effective identifier and also a partial representation. The difference is particularly clear for systems including metals

These two similar nickel complexes are effectively differentiated by InChI v1.06 so it is a good identifier

Treating the InChI as a representation also differentiates the structures, but loses information

The change in nickel geometry probably reflects a change in the electronic state of the nickel, which is very sensitive to the ligands

InChI v1.06

layered construction

InChI=1S/C5H10O2/c1-3-4-5(2)6/h3-6H,1-2H3/s4-3v/5-5/m0/s1

version/formula/connections/hydrogens/stereochemistry

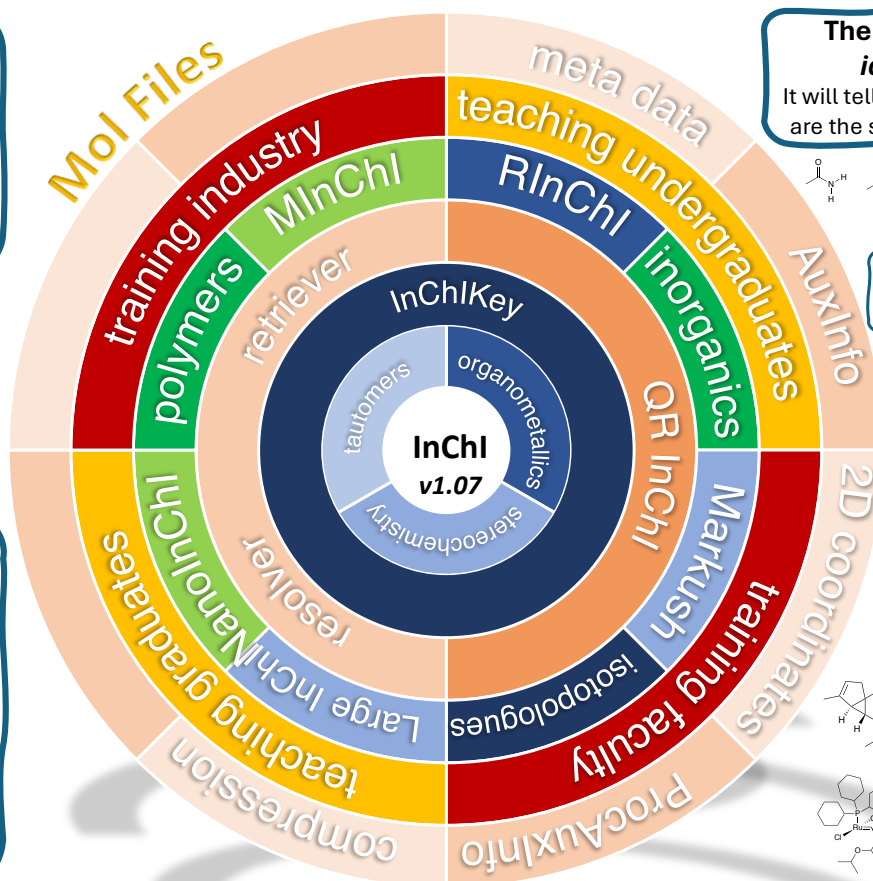
Try it out with the new Web Demo!

InChI v1.07
Try it now!

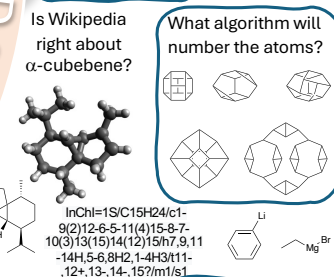
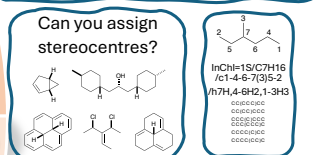
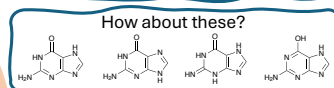
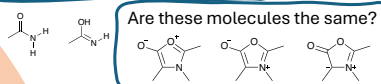
<https://iupac-inchi.github.io/InChI-Web-Demo/>

Join the discussion on:
<https://github.com/IUPAC-InChI/InChI/issues>

InChI can also be installed in a Docker container. The files for this are included in the release:
<https://github.com/IUPAC-InChI/InChI/releases/INCHI-1-TEST.zip>

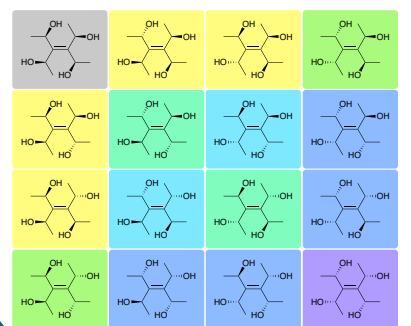


The InChI is an **identifier**
It will tell you if molecules are the same or different



The InChI is also a **partial representation**
You can often reconstruct a structure from an InChI

How many stereoisomers for 3,4-bis(1-hydroxyethyl) hex-3-ene-2,5-diol?



References:

- InChI Source Code: <https://github.com/IUPAC-InChI/InChI>
- J. M Goodman, I. Pletnev, P Thiessen, E. Bolton and S. R. Heller. InChI version 1.06: now more than 99.99% reliable. *J. Cheminform.* 2021, **13**, 40.