InChI: what is it and what will it be?

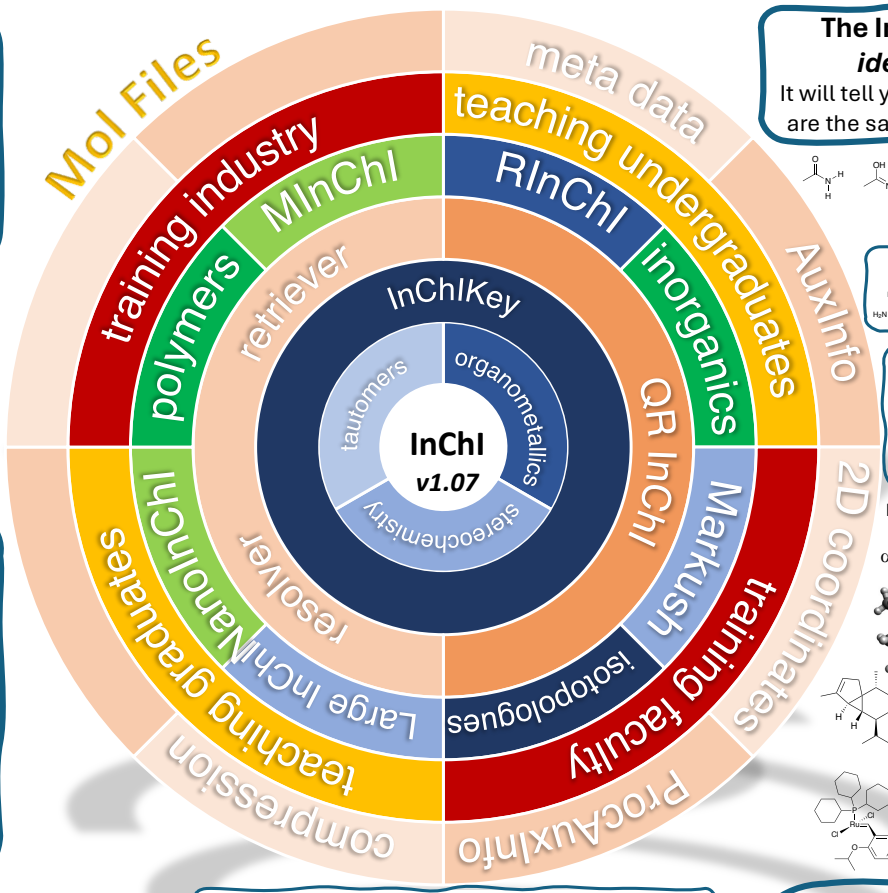
Gerd Blanke,[1] Jonathan M. Goodman[2]

1. StructurePendium Technologies GmbH, Essen, Germany;
2 Yusuf Hamied Department of Chemistry, University of Cambridge, CB2 1EW, UK

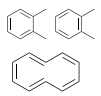
The InChI is the *international chemical identifier*, providing dependable, canonical names for molecular structures.

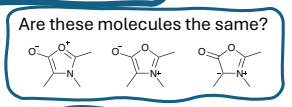
The latest release, InChI v1.07, [1] has security enhancements and refactored code, building on v1.06. [1]

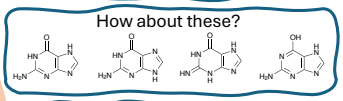
The code is all available on GitHub. [1]

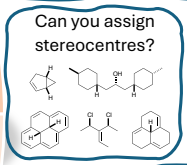


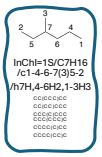
The InChI is an *identifier*
It will tell you if molecules are the same or different









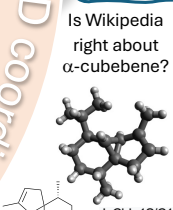


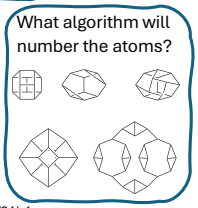
Work on the InChI continues

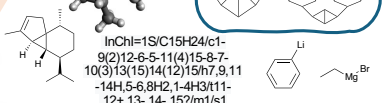
extended stereochemistry
tautomers
organometallics
molecular inorganics
polymers
nanomaterials
isotopologues
macromolecules

Applications are addressing new areas of InChI-based data-handling.

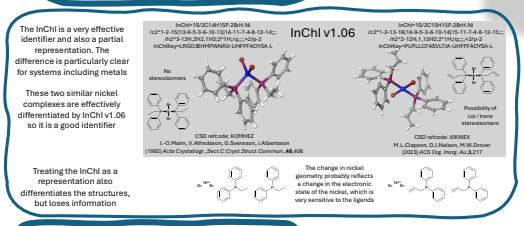
Mixture-InChI
Markush-InChI
Nano-InChI
Reaction InChI







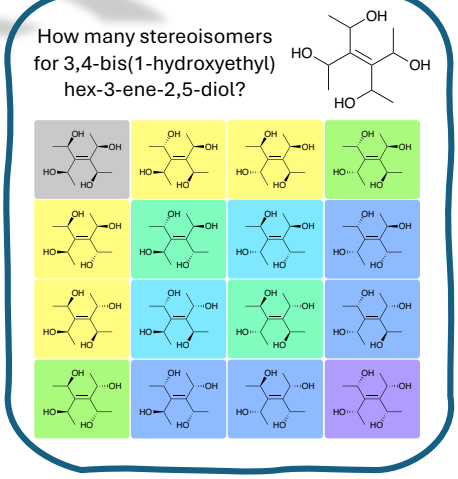
The InChI is also a partial representation
You can often reconstruct a structure from an InChI



layered construction

```
InChI=1S/C5H10O/c1-3-4-5(2)6/h3-6H,1-2H3/b4-3+/t5-/m0/s1
version /formula/connections/hydrogens /stereochemistry
```

How can the InChI help you?



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

References:

1. InChI Source Code: **https://github.com/IUPAC-InChI/InChI**
2. 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.