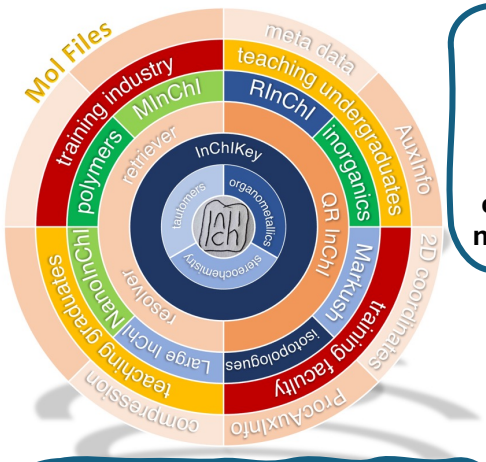
The InChI Today: is there anything it cannot do?

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

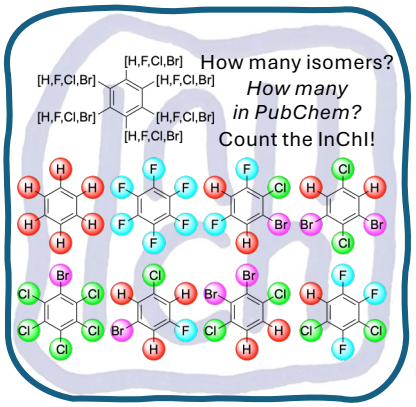
1. StructurePendium Technologies GmbH, Essen, Germany;
2 Yusuf Hamied Department of Chemistry, University of Cambridge, CB2 1EW, UK



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

The 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

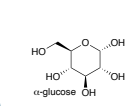


organometallic molecules

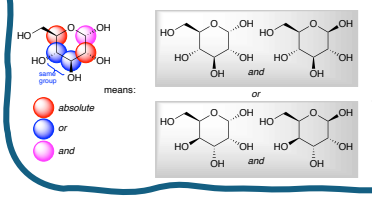
Where are the bonds?

- InChI v1.07.5: bonds to metals are broken
- InChI development version: bonds are broken only when there is a high electronegativity difference between the terminal atoms

enhanced stereochemistry

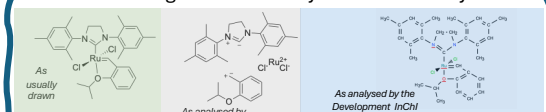


It would be helpful to have an InChI for racemic mixtures, other more complicated stereochemical mixtures, and to express uncertainty. The *Biovia* v3000 molfile can describe *enhanced stereochemistry*. Stereocentres or groups of stereocentres can be marked as ***absolute***, ***or*** (the configuration drawn or the inverse), ***and*** (the configuration drawn and the inverse). This is now being added to the InChI and is available in the web demo.



Soon:
atropisomers and stereochemistry through conformational restriction

The second-generation Hoveyda-Grubbs catalyst

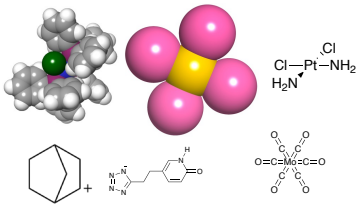


InChI=1S/C21H26N2.C10H12O.2ClH.Ru/c1-14-9-16(3)20(17(4)10-14)22-7-8-23(13-22)21-18(5)11-15(2)12-19(21)6;1-8(2)11-10-7-5-4-6-9(10)3;;;/h9-12H,7-8H2,1-6H3;3-8H,1-2H3;2*1H;/q;;;;+2/p-2

InChI=1B/C31H38Cl2N2ORu/c1-20(2)36-28-12-10-9-11-27(28)19-37(36,32,33)31-34(29-23(5)15-21(3)16-24(29)6)13-14-35(31)30-25(7)17-22(4)18-26(30)8/h9-12,15-20H,13-14H2,1-8H3

Both InChI are reasonably good identifiers;
the new one includes the bonds to ruthenium and so is a more discerning identifier and an improved representation

Can you think of a molecule that the InChI will find difficult?



Send us your ideas using the web demo https://iupac-inchi.github.io/InChI-Web-Demo/

IDENTIFIERS

The InChI
Chemical Identifier

Application InChIs
InChI-based techniques

descriptors

Reaction InChI

Polymer InChI

Mixture InChI

Nano InChI

What next for the InChI?

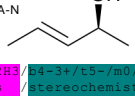
InChI v1.07.5

Try it now!

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

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

(*S*,*E*)-pent-3-en-2-ol
InChI=1S/C5H10O/c1-3-4-5(2)6/h3-6H,1-2H3/b4-3+/t5-/m0/s1
InChIKey=GJYMQFMQRRNLCY-BHYDHMSTSA-N



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

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.

We thank the InChI Trust and all other InChI supporters