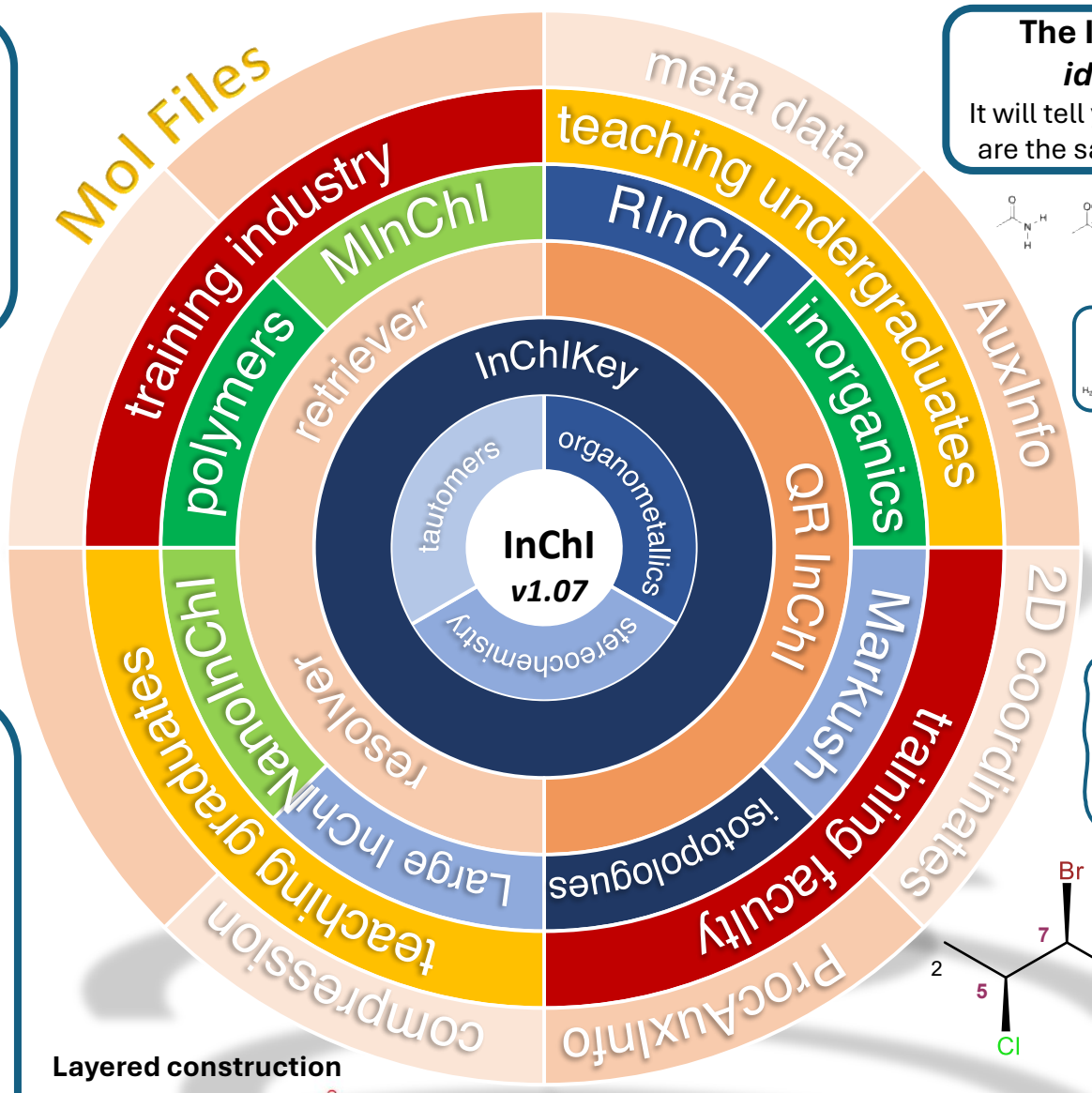
InChI: what is it and what will it be?

Gerd Blanke,[1,2] Jonathan M. Goodman[3]

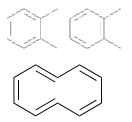
[1] InChI Trust, Cambridge, UK; [2] StructurePendium Technologies GmbH, Essen, Germany
[3] Yusuf Hamied Department of Chemistry, University of Cambridge, CB2 1EW, UK

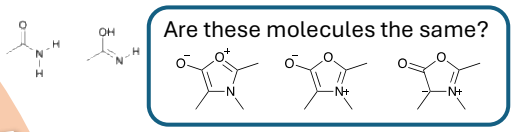
The InChI is the *International Chemical Identifier:* dependable, canonical names for molecular structures.

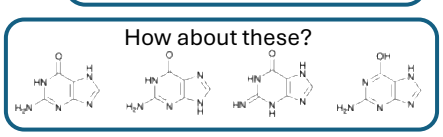
The latest releases, InChI v1.07, [1] have security enhancements and refactored code, building on v1.06. [2] , beta versions are coming out for molecular inorganics and MDL enhanced stereochemistry
New software version system: year.release_id, e.g. 2026.1

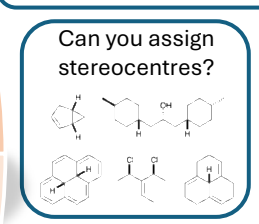


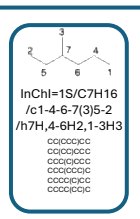
The InChI is an *identifier*
It will tell you if molecules are the same or different



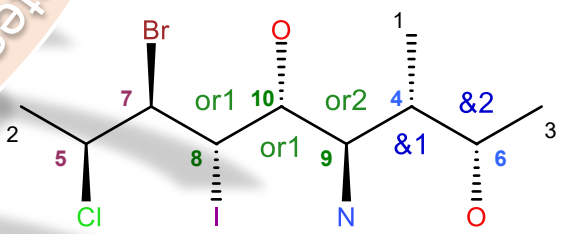








New: Support of MDL enhanced stereochemistry



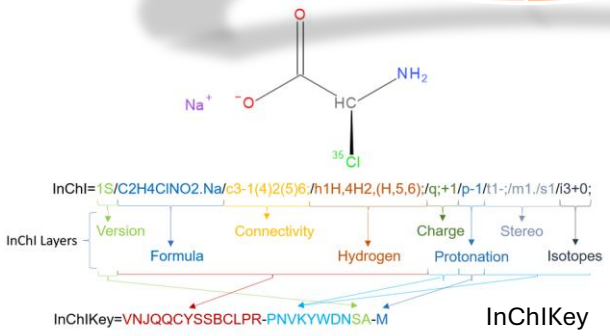
Work on the InChI continues

extended stereochemistry
tautomers
organometallics
molecular inorganics
polymers
nanomaterials
isotopologues
macromolecules

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

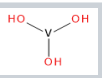
Mixture-InChI
Markush-InChI
Nano-InChI
Reaction InChI

Layered construction



InChI=1B/C10H20BrClNO2/c1-4(6(3)15)9(14) 10(16) 8(13)7(11)5(2)12/h4-10,15-16H,14H2,1-3H3/t4-,5-,6-,7+,8-,9,10+/m1/s1(5,7)2(8,10)(9) 3(4)(6)

New: Bond handling of molecular inorganics

Structure	Standard InChI	Transformation	Mol. Inorganics new standard InChI	Comments
	InChI=1S/3H2O.V/h3*1H2;/q;;;+3/p-3		InChI=1BI/3H2O.V/h3*1H2;/q;;;+3/p-3	ΔEN (O-V) >= 1.7, disconnect bond
	InChI=1S/3FH.V/h3*1H; /q;;;+3/p-3		InChI=1BI/3FH.V/h3*1H;/q;;;+3/p-3	ΔEN (F-V) >= 1.7, disconnect bond
	InChI=1S/3ClH.V/h3*1H; /q;;;+3/p-3		InChI=1BI/Cl3V/c1-4(2)3	ΔEN (Cl-V) < 1.7, keep bond
	InChI=1S/FH.O.V/h1H;; /q;;+1/p-1		Old: InChI=1/FH.OV/c;1-2/h1H;/q;+1/p-1 New: InChI=1BI/FOV/c1-3-2	ΔEN (F-V) >= 1.7 Org.: Break bond Fixed: V=O stops bond break between V and F
	InChI=1S/ClH.O.V/h1H;; /q;;+1/p-1		InChI=1BI/ClOV/c1-3-2	ΔEN (Cl-V) < 1.7 and V=O

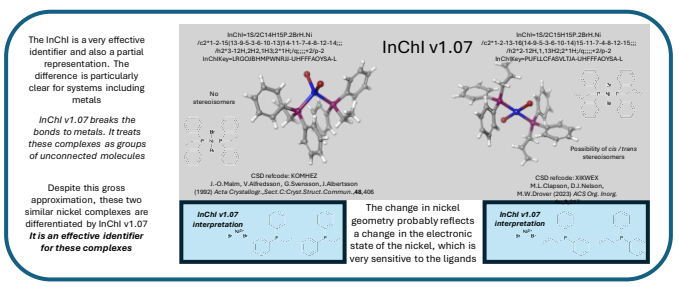
Current standard InChI deletes all bonds to metal atoms
New standard InChI only deletes the bonds under certain conditions: ΔEN >= 1.7 (related to Pauling rule; ΔEN electronegativity difference between two bonded elements) , double and triple bonds and bonds between H atoms and the metal atom are always kept. Only delete bonds if all bonds fulfill the deletion criteria.

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.

Try it out with the InChI Web Demo!
https://iupac-inchi.github.io/InChI-Web-Demo/

What is next?



Thanks to all InChI funders

BEILSTEIN INSTITUT
InChITRUST
VolkswagenStiftung