InChl for inorganic chemists: organometallics and molecular inorganics

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The standard InChI, v1.07, was developed with organic molecules as the focus. The algorithm generates InChI for organometallics which can be helpful as identifiers in an organic chemistry context, but which neglect important aspects of these structures. Filling these gaps is a priority. For example, the NFDI4Chem initiative (www.nfdi4chem.de) will use InChI for molecular inorganic

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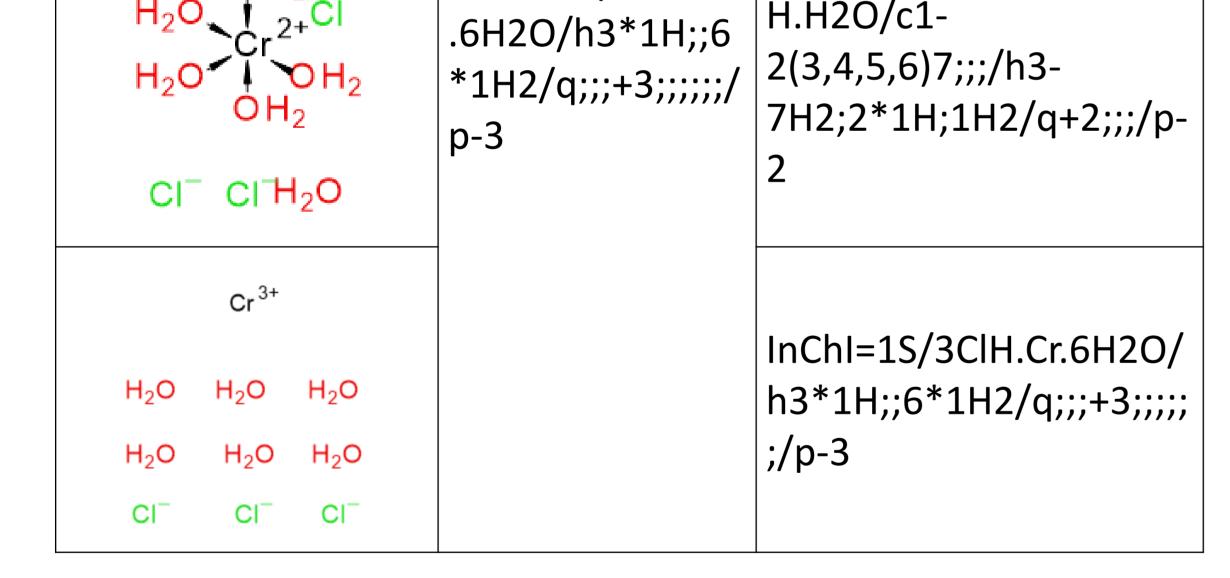
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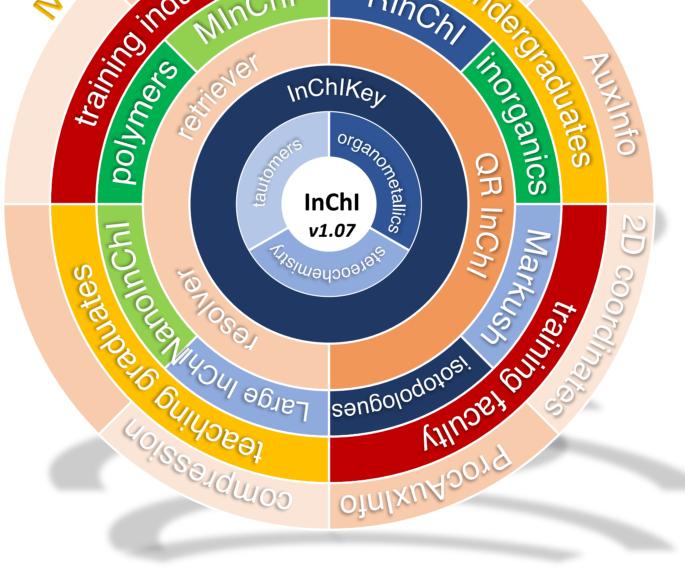
compounds as well as organic ones. A better description of organometallics is needed.

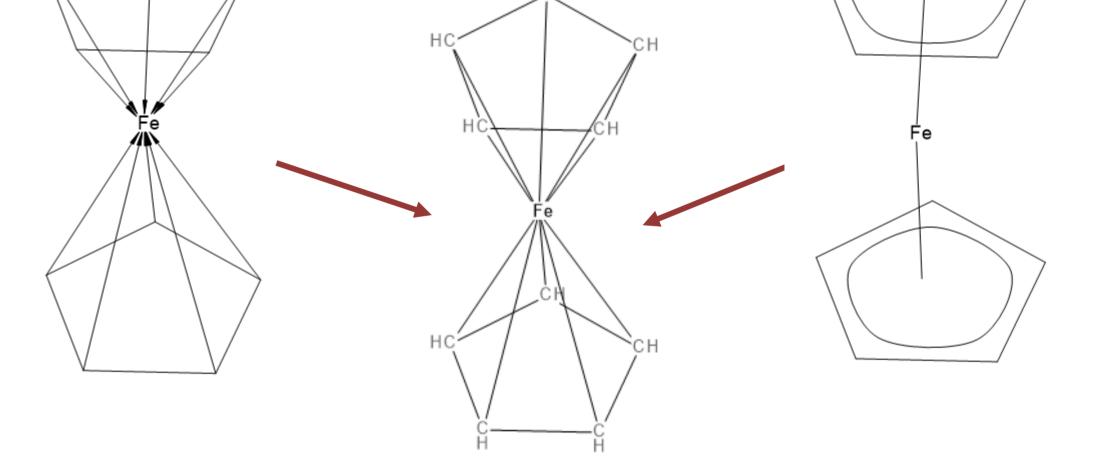
A revision of the InChI is being developed which includes more information about the organometallics and molecular inorganics. This requires an improved bond recognition and a more sophisticated stereochemical model.

Depiction	Current standard InChI (1.07)	Developing standard InChI
$H_2O + H_2O + $		InChI=1S/3ClH.CrH12O6 /c;;;2- 1(3,4,5,6)7/h3*1H;2- 7H2/q;;;+3/p-3
	InChI=1S/3ClH.Cr	InChI=1S/CICrH1005.2CI

A compound can only be identified by one InChI but may be represented by different structure diagrams. The new InChI program will interpret diverse diagrams of inorganics and organometallics. Structure depictions of the same compound may especially differ in the bond types used for the chemical representation. Beside single, double, and triple bonds, other bond types like coordinative or haptic bonds of the input structure depictions must be processed accordingly to ensure the creation of unique InChls. Hydrogen atoms directly bound to metal atoms must always be drawn explicitly. Guidance on constructing accurate diagrams will be available.







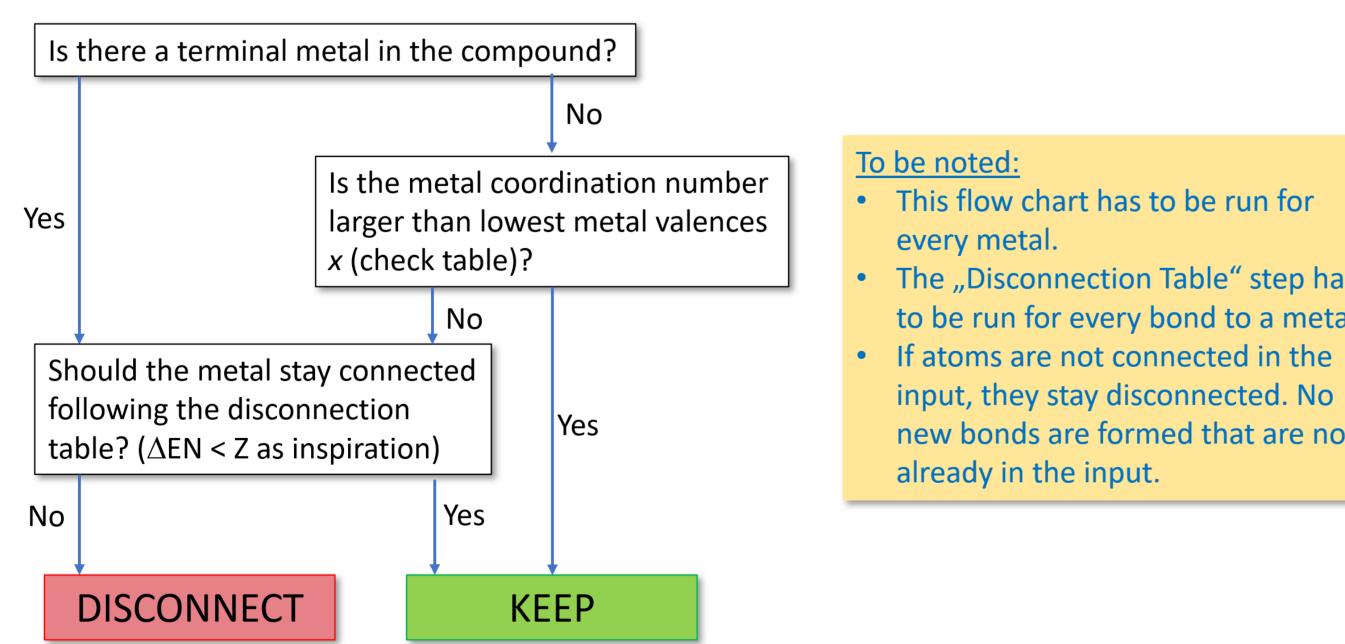
InChI=1/2C5H5.Fe/c2*1-2-4-5-3-1; /h2*1-5H;/rC10H10Fe /c1-2-4-5-3(1)11(1,2,4,5)6-7(11)9(11)10(11)8(6)11/h1-10H

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

The stereochemistry recognition of InChI must be extended to the more complex relationships in inorganic compounds. While tetrahedral stereocentres may lead up to 2n stereoisomers (with n = number of stereocentres), just one octahedral centre leads up to 30

The standard InChI, v1.07, breaks all bonds to metal atoms; the new standard InChI will be more selective. A data-driven approach will be used to decide whether bonds to metals should be retained.

Preprocessing flow chart for inorganic compounds



The "Disconnection Table" step has to be run for every bond to a metal. new bonds are formed that are not

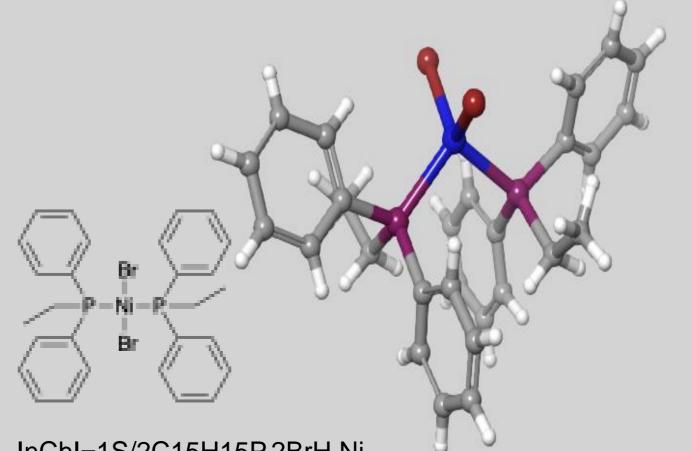
Test the InChl developments

References:

1.InChI Source Code: https://github.com/IUPAC-InChI/InChI 2. Making the InChI FAIR and sustainable by moving to opensource on GitHub: https://chemrxiv.org/engage/chemrxiv/ article-details/66a9584301103d79c547b086

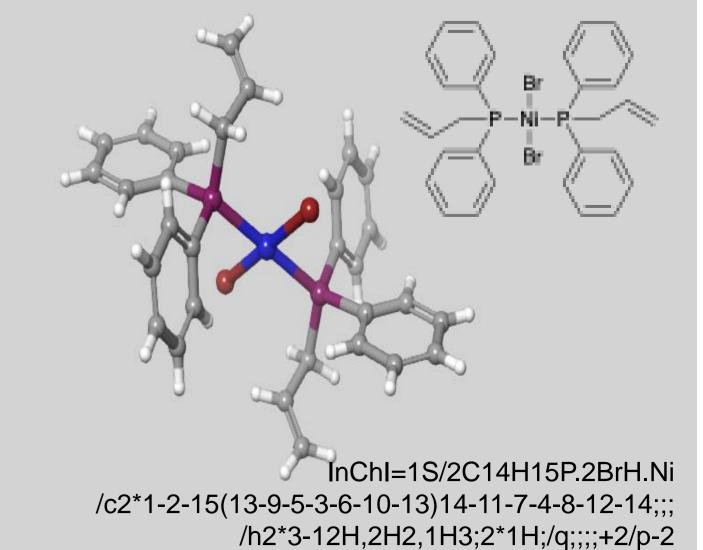
isomers.

Tetrahedral No stereoisomers



InChI=1S/2C15H15P.2BrH.Ni /c2*1-2-13-16(14-9-5-3-6-10-14)15-11-7-4-8-12-15;;; /h2*2-12H,1,13H2;2*1H;/q;;;;+2/p-2

Square planar Possibility of *cis / trans* stereoisomers



CSD refcode: XIKWEX, M.L.Clapson, D.J.Nelson, M.W.Drover (2023) ACS Org. Inorg. Au, 3, 217