

IUPAC InChI - Recent Developments in The

Worldwide Chemical Structure Identifier Standard

Stephen R Heller^{1,2}, Gerd Blanke^{1,5}, Ian Bruno^{1,2,3}, Jonathan M Goodman^{2,6},
Richard Kidd^{4,1} and Rudy Potenzone¹,

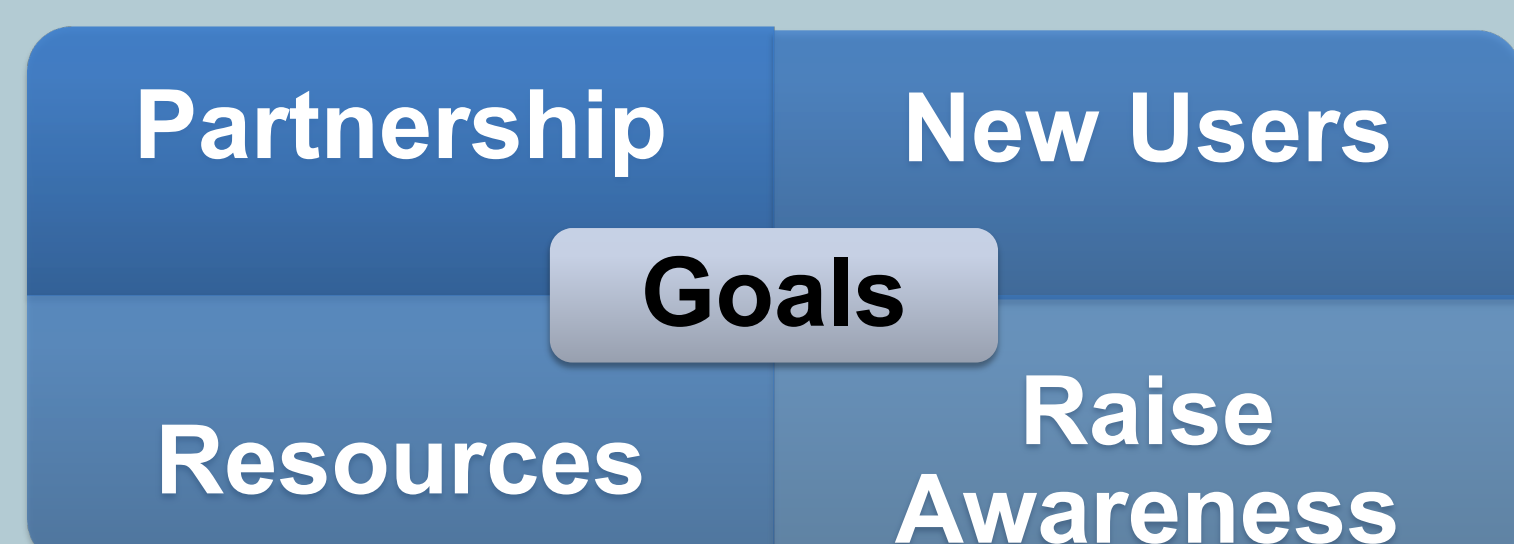
¹InChI Trust; ²IUPAC; ³ Crystallographic Data Centre (CCDC); ⁴Royal Society of Chem; ⁵StructurePendium Tech; ⁶Yusuf Hamied Dept Chem, U of Cambridge

InChI Project Goals

Create a **free, non-proprietary chemical substance identifier**:

Turn chemical structures into unique, canonical text strings
Enable easier finding and linking of chemical and biological data

- Collaboration and partnerships
- Educational resources



- Raise awareness
- Collaboration and partnerships

InChI Supports the FAIR Project

- Findability, accessibility, interoperability, and reusability
- In particular– **findability** and **reusability**
- The first step in (re)using data is to find and link it
- InChIs allow **interoperability** between structures and related (meta)data including qualified references to other (meta)data

InChI is critical to enable references based on chemical identity

We address this global challenge with international cooperation and support the needs of industry, academia, governments and individuals

Examples of InChI Adoption

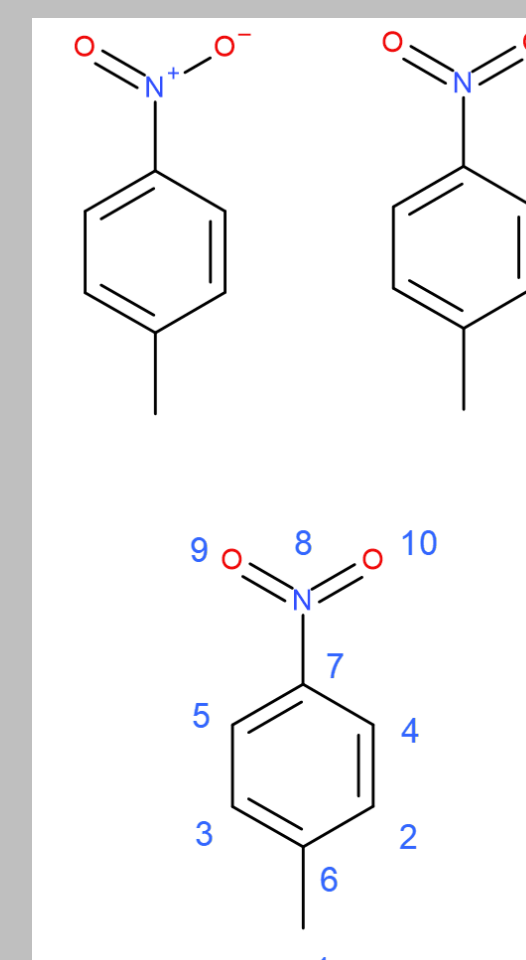
Databases

Elsevier/Reaxys –179 million
EBI UniChem –177 million
NIH/NCI/CADD/iRL – 140 million
RSC/ChemSpider –114 million
NIH/PubChem - 111 million
Chemical Abstracts Service – 264 million

Virtual repositories

GDB17 (The Human Genome Database) –166 Billion
NIH/NCI/Argonne/SAVI – 1.75 Billion

InChI and InChIKey



InChI: are built to work as a chemical identifier
Different representations can lead to one InChI

InChI= 1S (InChI version 1, Standard)
/C7H7NO2 (Formula C: 1-7, N:8, O: 9-10)
/c1-6-2-4-7(5-3-6)8(9)10 (Connectivity)
/h2-5H,1H3 (Hydrogen layer)

InChI = 1S/C7H7NO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5H,1H3

InChI Version

Formula C: 1-7, N:8, O: 9-10

Connectivity

Hydrogen layer

InChIKey: Fixed-length hash of InChI: identity and web searches

InChIKEY= ZPTVNYMJQHSSEA (formula, connectivity, hydrogens (hashed))
UHFFFAOY (remaining layers: stereochemistry, isotopes, etc. (hashed))
SA (Standard InChI, version 1 (= A))
N (Neutral / total charged atoms)

InChIKey = ZPTVNYMJQHSSEA-UHFFFAOYSA-N

Formula and connectivity hashed

Stereochemistry etc. hashed

InChI Version

Neutral or charged

InChI Trust Financials

- Core revenue \$160k from Member fees
- Revenue has been enough for core maintenance and minimal incremental expansion and outreach
- The current budget is by far not sufficient for the current urgent enhancements: stereochemistry extensions, organometallics, tautomers, epitopologues, etc.

InChI Working Groups

- Extended Stereochemistry
- Extended Tautomers
- Isotopologues
- Large Molecules
- Monomer Atoms
- Organometallics/Inorganics
- Variable Structure (Markush)
- GitHub code development
- Mixtures
- Nanomolecules
- QR Codes
- Open Education Resource (OER)
- Reactions
- Resolver

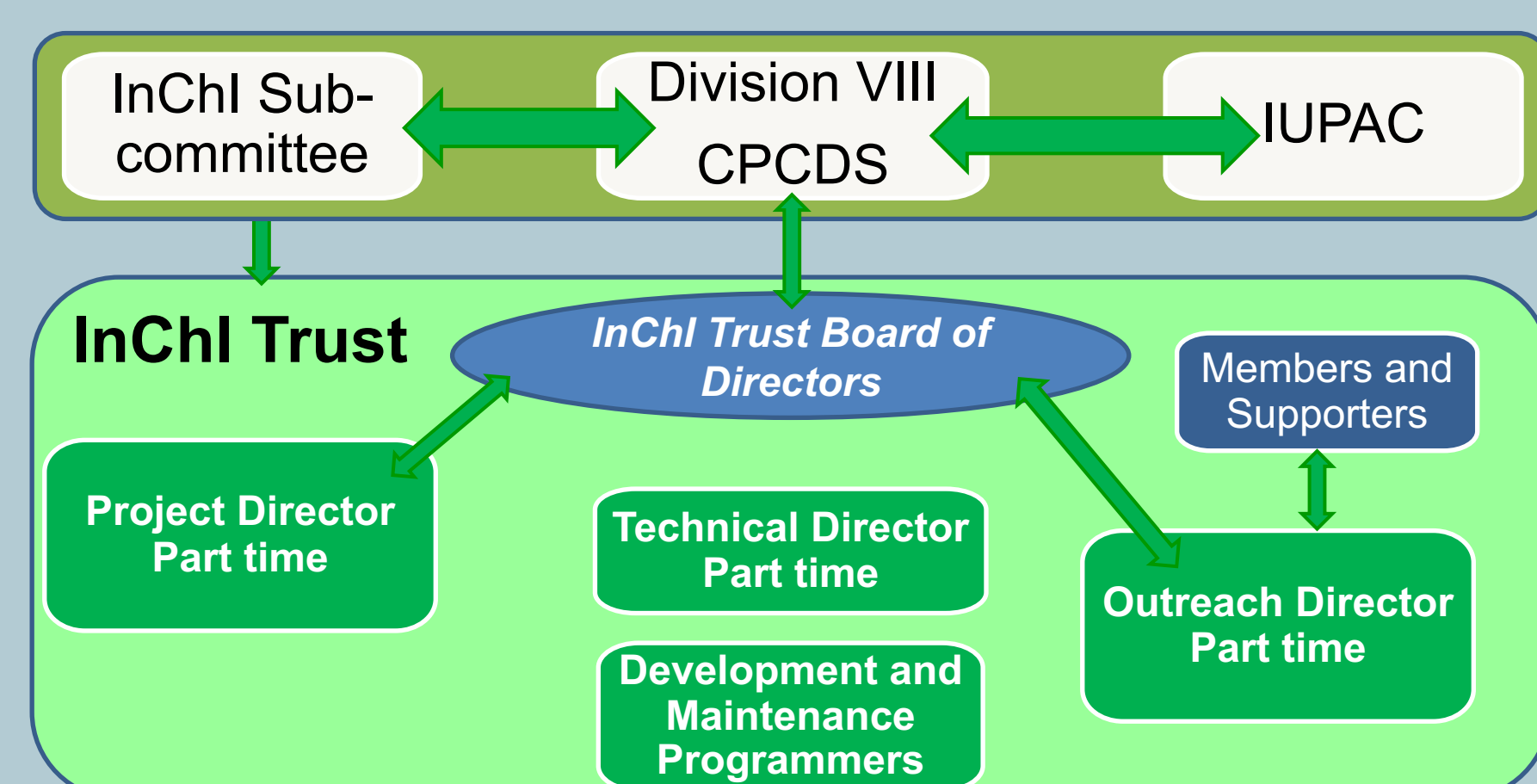
InChI release status: <https://github.com/IUPAC-InChI>

InChI versions:

Released
Current version 1.06
<https://www.inchi-trust.org/downloads>
https://github.com/IUPAC-InChI/InChI_1_06
Latest implemented enhancements
Polymers (in beta status)
Under development
Requirements (nearly) ready
Organometallics
Stereochemistry
Tautomers
Isotopologues
Full V2/V3 molfile support (for registration)
Sgroups and Sgroup data
Longer evaluations
Large molecules
Variable molecules / Markush InChIs

Applied InChI versions:
Released
RInChI 1.0
Test Phase
Resolver
<https://github.com/inchiresolver/inchiresolver#readme>
0
QR code
RInChI 1.1
Test phase: <https://github.com/IUPAC-InChI/RInChI>
Awaiting coding
MInChI
Prototype released:
<https://github.com/ccd/mixtures>
RInChI (1.2)
Atom mapping
Under development
NanoInChI (NInChI)

InChI Organization



InChI Trust Was Created to Oversee InChI

- UK Public Benefit Charity
- The Trust has 15 Members who renew annually and pay an annual fee



InChI Future

Support the further InChI development

- Contribution in kind based on the open-source development on GitHub
- Donations to the InChI-Trust
- Cooperation with InChI-Trust certified consulting companies

If you are interested to participate in the further InChI development become a member of the InChI Trust