InChI is...

InChI is the IUPAC International Chemical Identifier (InChI).

- A unique identifier for a chemical structure.
- Universally available chemical identifiers.
- A human readable string of characters derived directly from a structural representation of a chemical substance.
- A project of IUPAC and the InChI Trust.

The purpose of InChI is...

- To streamline naming conventions for chemical components and reactions.
- To uniquely identify a chemical substance, without ambiguity, providing a precise, robust, structure-derived tag for chemical substances.
- To assist in merging and linking chemical databases.

InChI is essential...

As the only structure representation standard in the public domain, open-source and freely available to the scientific community.

The InChI Timeline

1999/2000 Steve Heller and Steve Stein initiate the InChI project at the request of IUPAC.
2005 Launch of InChI.
2008 A fixed length (27 character) condensed digital representation of the InChI called the InChIKey was developed.
2009 Formation of a Trust for a strategic vision and funding for the InChI project.
2017 Latest version of the InChI software was internally aligned, with InChI-1b for inorganic compounds.
2019 InChI-1c released.

And still more to come...

The InChI project is ongoing; not all of chemistry is yet covered by the software. The vast majority of organic compounds can be encoded into InChIs, but many inorganic and organometallic compounds are still work in progress.

Make your own

The key component of InChI-enabled communication is a software package that encodes a chemical structure into a string of letters and numbers called an identifier. The InChI software in action.

- If both sender and receiver have the InChI software, they can:
  - Communicate chemical structures simply by encoding the structure into the string using the free software tool, transmit the unique identifier.
  - The receiver then decodes (with the identical software) the string back into a connection table.

Learn more here

Videos by the InChI Trust:
- YouTube: youtube.com/watch?v=mpZj4b9elYE

InChI page on IUPAC:
supra-agents.org/inchi/identifiers.html