Improvements in InChI treatment of stereoconfiguration

Results of discussion - decisions, proposals and plans

Status and Future of the IUPAC InChI: context and use cases

August 16-18, 2017, NIH, Bethesda, US

Stereo - Decisions and plans

1. Enhanced Streoconfiguration definition in MOL V3000.

Mostly agreed that we should consider support of enhanced stereo. First step will be draft document describing this concept with relevant examples accompanied with corresponding sets of stereoisomers implied.
Andrey Yerin, John Mayfield.

Discussion of this document with 'stereochemistry group' and especially InChI developers.

Proposal is made: After the first document consider a possibility to write a paper for PAC describing the concept of 'enhanced stereo definition' and consider its implications and relation to chemical nomenclature.
Specifically about citation of relation between RS/SR and R*/S*.

Work for a team composed of "InChI stereo" and Division VIII representatives.

Such paper can formally validate the concept and merge nomenclature and electronic representation conventions.

Stereo - Decisions and plans

2. Cummulenes

InChI code intentionally restricts the length of allenes for detection of stereoisomers. Check InChI Manual. Can be extended. Prevailing opinion is no restriction necessary.

(Let them tire drawing what we do not support. 10-20??)

3. Atropisomerism

Specify principles and cases to support, expected procedures and algorithms. Consult InChI Manual and propose new type(s) of supported stereogeneic units.

Specification of atom nature, bond types, cyclicity is expected to define the cases where such stereo exists. Proposed to keep stereo indication in 't‘ layer.

Andrey Yerin + ?

Stereo - Decisions and plans

4. Haworth and other specific representations.

Possibility to recognize configurations and generate correct InChIs.

Current opinion is that some external application converting Haworth and perspective representations to explicit representation can be used. Will be discussed further.

Karl Nedwed presentation, a possibility to have access to such tool and integrate or develop something close for InChI tools.

5. Recognition of wrong arrangements.

Check InChI Manual and look for restrictions and propose new cases to refuse.

Stereo - Decisions and plans

6. Support of stereo in non-tetrahedral arrangements.

Longer task than any above. Needs consideration of conditions to recognize isomerism.

For 2D all agreed that we should start any stereo considerations once we have at least one stereobond at the center. Next considerations of atom type and specific configurations.

For 3D it simpler but algorithms are necessary to get configuration descriptor.

The task can be done in collaboration with coordination and organometallic group where non-tetrahedral configurations are important.

No one is responsible yet.

Stereo - Decisions and plans

Preliminary priority of tasks - should be discussed further:

Atropisomers and Haworth

Enhaced stereo representation (MOL V3000)

Non-tetrahedral stereo and bad representations

Longer cummulenes

The group should be established

Everyone interested in this work as a group member please indicate you interest – via InChI Trust, InChI Discuss forum or other