Treatment of polymers by InChI tools

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

Polymers – Decisions, proposals and plans

1. Hydrogen as end-groups

General decision is that we need this possibility.

Developers stated that it is not so difficult and can be included in (some) update.

2. Canonicalization with specified end groups

Also desirable.

The cost will be lost relation between encoding of CRU in a polymer with and without end-groups.

Should be considered as soon as normalization (phase shift) should change end-groups

Polymers – Decisions, proposals and plans

3. Folding – simplification of CRU

Probably desirable. Again has consequences – should be discussed.

4. Degree of polymerization and other related data

No agreement. Is it a kind of metadata? It is obviously a part of structural information, still can be added as additional search condition.

5. End-groups encoded in some separable way

No agreement. Some people would like to have it. Considerations necessary.

Polymers – Decisions, proposals and plans

6. Any special cases

Linkers, branching. How to represent? Examples are badly needed.

7. Some at least discussion group should be established

Who is going to participate?

Who is ready to provide examples?

Proposal to ask Polymer Division for anybody interested