InChI v. 1.06 pre-release

checklist

# Work - polymers

Issue #1 (in-SRU repeats, e.g. polyethylene vs. polymethylene)

Issue #2 (SRU canonicalization for non-star ends)

0D coords – what’s with FoldCRU? With FrameShift?

3D coords – what’s with FoldCRU? With FrameShift?

FoldCRU with non-bistar CRU’s?

In "/z" layer: change global-cano nums to #component:#local cano nums?

(local == in-component, global == whole-multicomponent-molecular-assembly);

then specifically take care on inchi2struct.

winchi-1 makes mistake on PEX#71 (keeps "4Zz" at the end of brutto-formula)

Gerd Blanke comments

Other feedback

# Work - multi-threading

Connect to & collaborate with Carl Nedwed

Add custom allocator stuff

Drop-in replacement for calloc/malloc/realloc?

# Work – bugfixes for “hard” bugs

Crash/hang/no-InChI hard bugs

Stereo related

Normalization related

PubChem BNS\_OVFL issue

Renumbering issues - small molecules

In PubChem (small molecules ) - PubChem renumbering miltiple issues

Renumbering issues – proteins and other large molecules

PDB (large molecules)

# Work – bugfixes for “security” bugs

v. 1.051 for Google (‘GAF’)

The next bug from Google (‘OnemoreGAFIssue’)

Cure53 bugs

# Work – bugfixes for SourceForge bugs

\*\*T114\*\* SourceForge #14 Preprocessing depends on order atoms are defined (Timo Boehme)

\*\*T115\*\* SourceForge #15 Different InChIs generated if atoms are swapped in a bond

\*\*T118\*\* SourceForge #18 Different InChIs dependent on atom input order (Daniel Lowe)

\*\*T119\*\* SourceForge #19 Error in auxinfo original atom order when hydrogen isotopes present

# Work – bugfixes for other bugs

test\_ixa on rtrip seems to read AuxInfo if supplied -- but does not read/use coordinates;   
also garbage appears in AuxInfo after i2s conversion

Bug or feature? IXA\_API does not read InChI when it's paired with AuxInfo, as Istvan from ChemAxon (?) noted... It is due to internal use of CheckINCHI() which does not pass some Auxinfo symbols. Is it OK? It effectively hides some dirty things with readi

#2: InChI software (Library called via API) hangs on some molecule

Curious behavior with stereo P (Burt Leland reported)

1.05 alias expansion bug for PubChem SID 162170046 (also 162171235, 162171236, 162171238,162171239)

? Issue by Josef Ringgenberg 2019-08-26 – inconsistent way of treating oxyhaloacids

# Non-bug issues

IXA Create atom/bond/stereo performance (Daniel Lowe)

Create optional (but StdInChI!) switch to relax control of stereocenter perception at alpha~180o (Yu. Borodina)

# Optional improvements & fixes

Polymers: AuxInfo->InChI for polymers

Polymers: Enable (H,H) for SRU, in addition to (\*, \*)

Polymers: Attachment points (M APO in ctab) are not handled but could be used   
in place of star atoms (John May)

Polymers: \*\*T014\*\* Recognize polymer SRU even if no SBL line [by bonds to \* and in src-based form] (Andrey Erin)

\*\*T012a\*\* Update the “UNDERIVATIZE” part to the code I gave to you previously? (DT on 2016-10-06)

\*\*T006\*\* Return #define INCHI\_DECL \_\_stdcall for Win32 dll, as per ACD/Labs request "for back-compatibility" (D. Redkin)

# Product backlog

\*\*T011\*\* InChI error examples - Burt Leland "for your backlog" (round-tripping through ChEMBL-18)

V3000 - presence of empty {M V30 BEGIN BOND/M V30 END BOND} block at count of bonds=0 emits error "No V3000 CTAB end marker"

#28: INCHIGEN-based API - add polymer treatment BACKLOG

#30: InChI 1.05 - problem with /Tabbed option BACKLOG

#31: \*\*T026\*\* Check Keith Taylor's: "large poynucleotide caused a crash. I cannot remember if this was the previous result." BACKLOG

#32: \*\*T009b\*\* Remaining minor issues on "Warnings during compilation (using gcc 6.2.1)", by Dominik 'Rathann' Mierzejewski BACKLOG

? #37: inchi2inchi for polymers - made work normally (currently a stub) BACKLOG

#38: Make all file reads (besides those V3000) via growing buffer rather than array{MAX...LEN] BACKLOG

Eliminating a non-stereo marked as stereo BACKLOG

#36: Bug reported by David Sharpe in [InChI-discuss] - "Double bond stereoperception dependant on precence of remote atoms with non-standard valence" BACKLOG

# Testing

Update ITS test set

Add polymers

Add large molecules

Burt Leland's suggestion (guaranteed-to-round-trip subset)

Regression tests

ITS (updated)

ChEMBL

PubChem

# Documentation

Release Notes

Update

Accept changes

Check and set the last date

Make PDF

TechManual

Update

Accept changes

Check and set the last date

Make PDF

User Guide

Update

Accept changes

Check and set the last date

Make PDF

API Description

Update

Accept changes

Check and set the last date

Make PDF

Readme in all sub-directories

Update headers

Update content

# Packaging

…

Here is …

…

…

…

Other comments if any

…

# TODO in last minutes

Remove all //

Remove #if 0

Remove temporary #ifdef (like UNCIVER\_OLD… or V106\_RENUM)

Remove TODO:

Update .rc (version info, etc.) in all programs

Comment out or remove all calls to debug macros ITRACE\_

Turn OFF engineering mode

At the end, prepare "Known bugs" list, if nothing other helps