

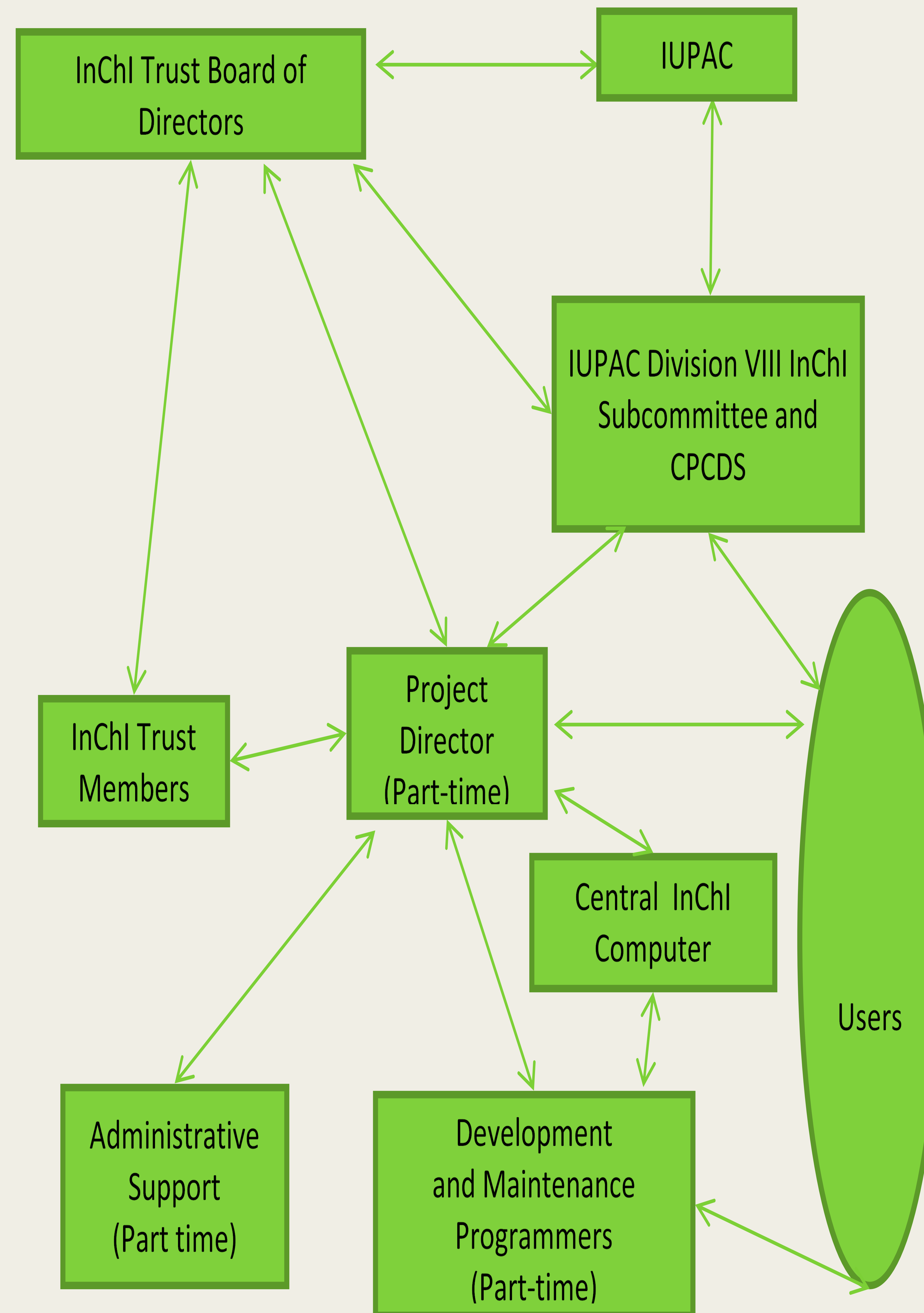
The Status of the IUPAC InChI Chemical Structure Standard – Today and the Future

Ray Boucher, Stephen Heller, and Alan McNaught

Objectives: Develop a computer algorithm to produce unique label – Chemical Identifier (InChI)

Create Open Source, non-propriety Identifier Used in printed and electronic source

Enable easier linking to diverse data and information compilations; Not a replacement for any existing internal structure representations



<http://www.inchi-trust.org>

Acknowledgements

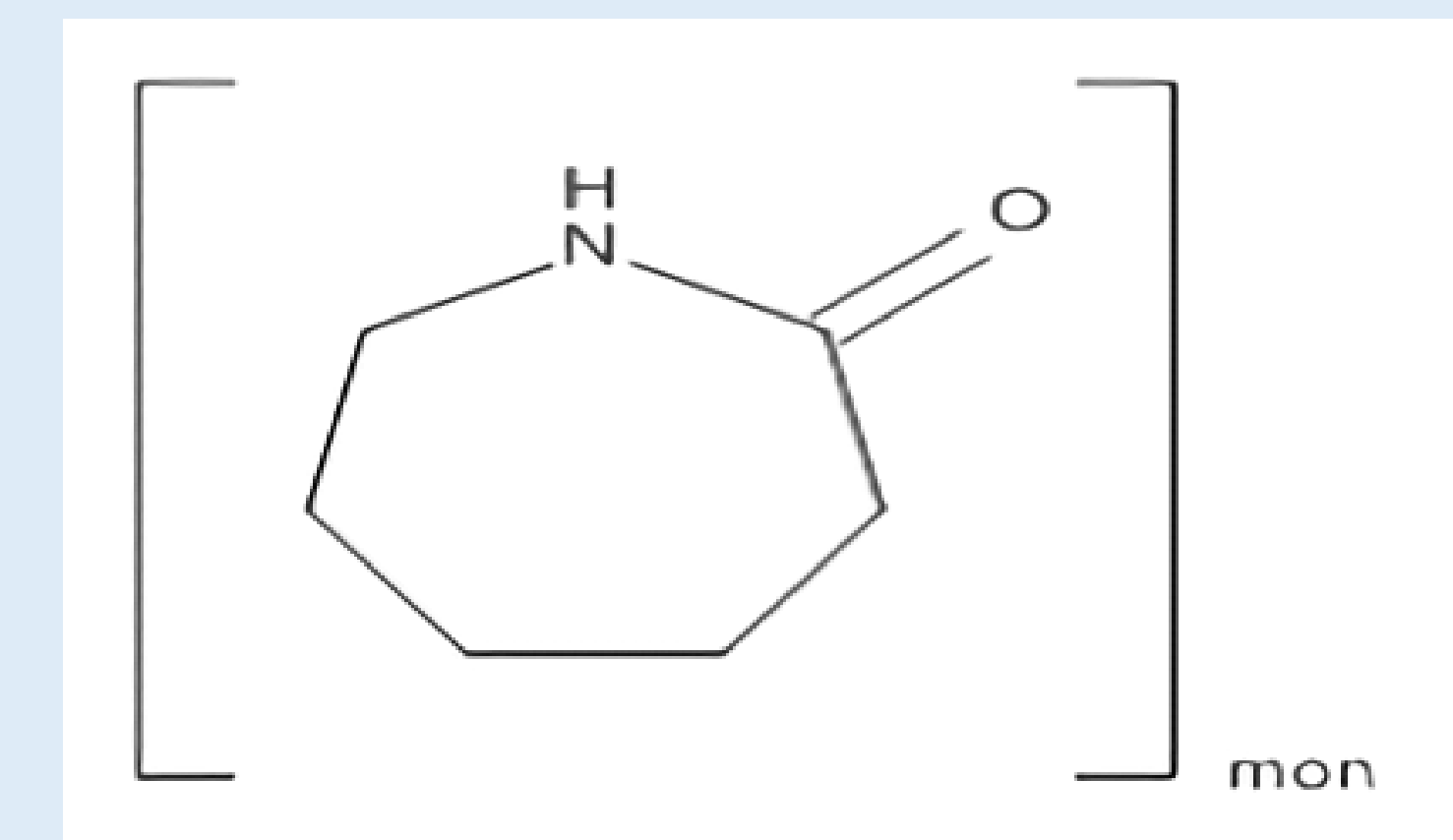
(Primarily members for the IUPAC InChI subcommittee and associated InChI working groups)

Steve Bachrach, Colin Batchelor, John Barnard, Evan Bolton, Steve Boyer, Ian Bruno, Steve Bryant, Dominic Clark, Szabolcs Csepregi, Rene Deplanque, Gary Mallard, Nicko Goncharoff, Jonathan Goodman, Guenter Grethe, Richard Hartshorn, Jaroslav Kahovec, Richard Kidd, Hans Kraut, Alexander Lawson, Peter Linstrom, Leah McEwan, Bill Milne, Gerry Moss, Peter Murray-Rust, Heike Nau, Marc Nicklaus, Carmen Nitsche, Matthias Nolte, Igor Pletnev, Josep Prous, Peter Murray-Rust, Hinnerk Rey, Ulrich Roessler, Roger Schenck, Martin Schmidt, Steve Stein, Peter Shepherd, Markus Sitzmann, Chris Steinbeck, Keith Taylor, Dmitrii Tchekhovskoi, Bill Town, Wendy Warr, Jason Wilde, Tony Williams, Andrey Yerin.

Special Acknowledgement: Ted Becker & Alan McNaught for their vision and leadership of the future of IUPAC nomenclature.

InChI for Polymers

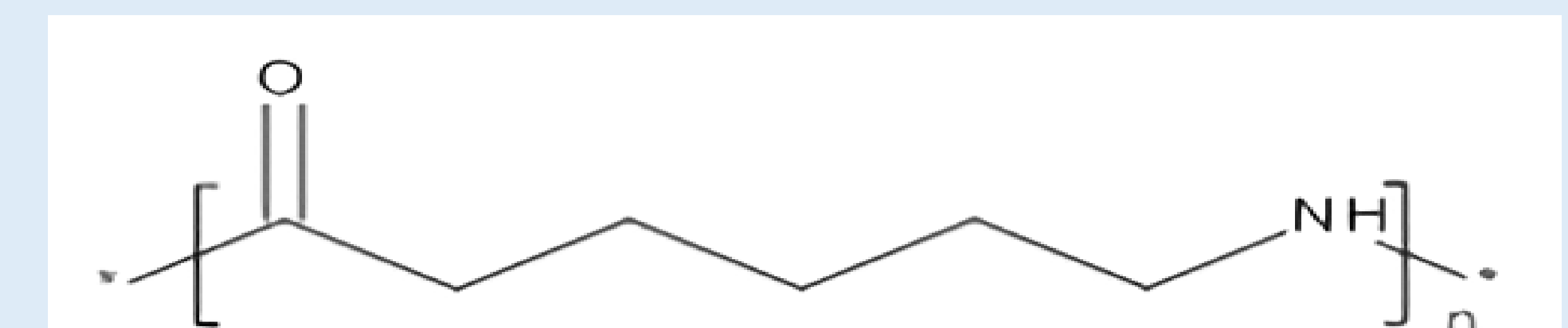
source-based, poly(caprolactam)



InChI=1B/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)/z200-1-8

InChIKey=JBKVHLHDHXXQEQ-ZMQGHSKBA-N

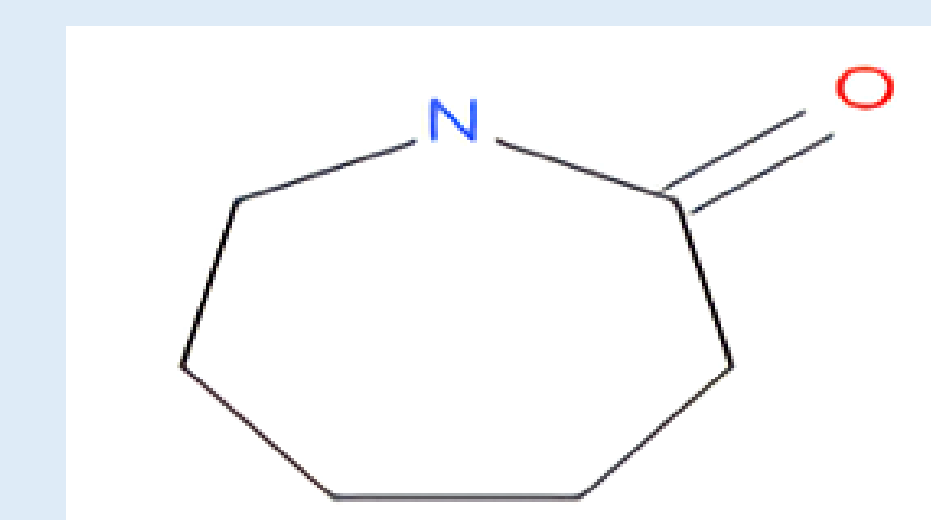
structure-based representation



InChI=1B/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)/z101-1-8(1,2,1,3,2,4,3,5,4,6,5,7)

InChIKey=JBKVHLHDHXXQEQ-DZWZRWJOBA-N

and single monomer, caprolactam:



InChI=1S/C6H11NO/c8-6-4-2-1-3-5-7-6/h1-5H2,(H,7,8)

InChIKey=JBKVHLHDHXXQEQ-UHFFFAOYSA-N

They have the same first part of InChI and 1st block of InChIKey!