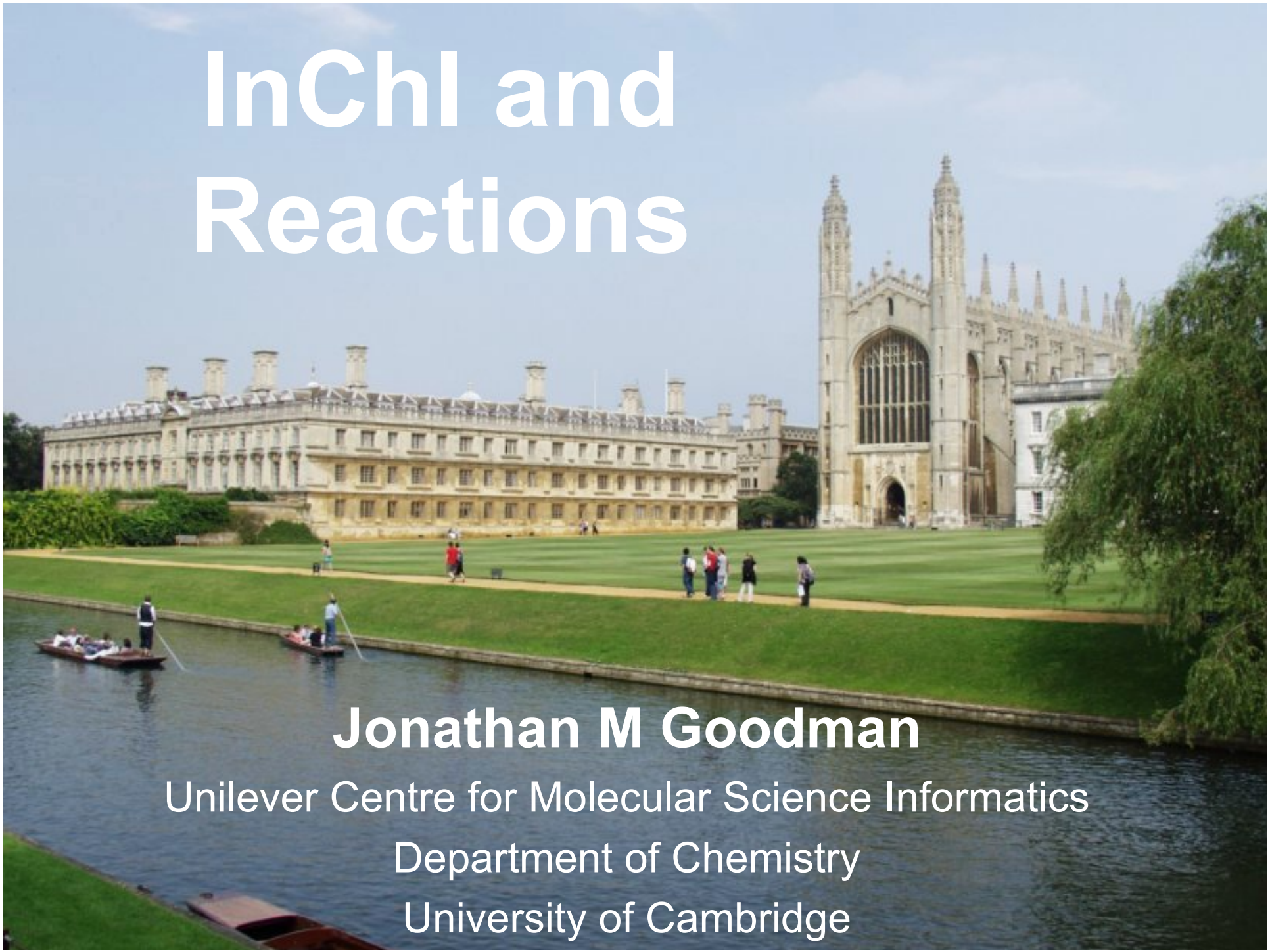
InChI and Reactions



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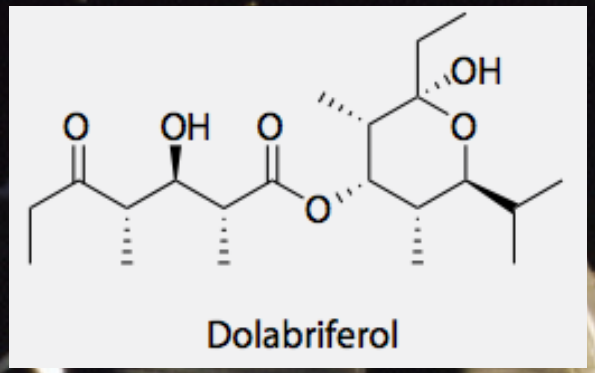
InChI and Reactions



Dolabriferol

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Department of Chemistry

University of Cambridge

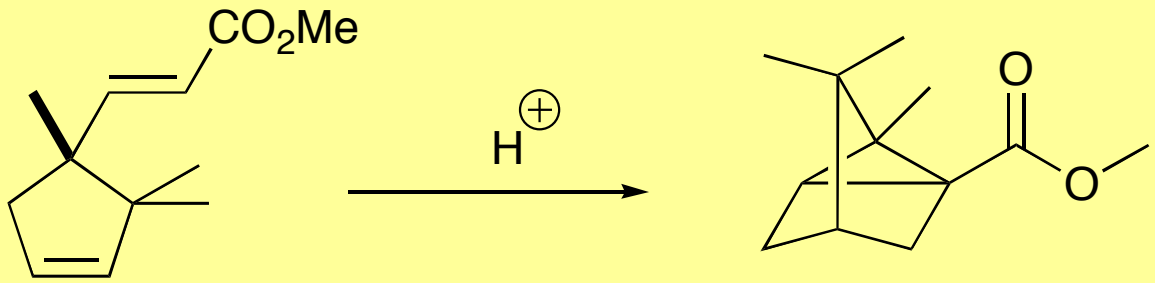
Solubility Challenge

Can You Predict Solubilities of Thirty-Two Molecules Using a Database of One Hundred Reliable Measurements?

A. Llinas, R. C. Glen, and J. M. Goodman

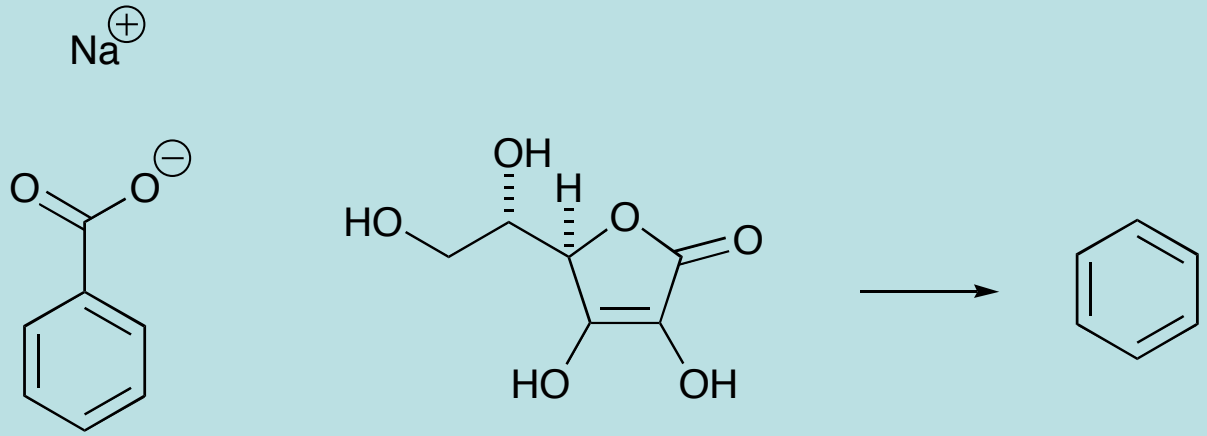
J. Chem. Inf. Model. 2008, **48**, 1289-1303.

No literature data



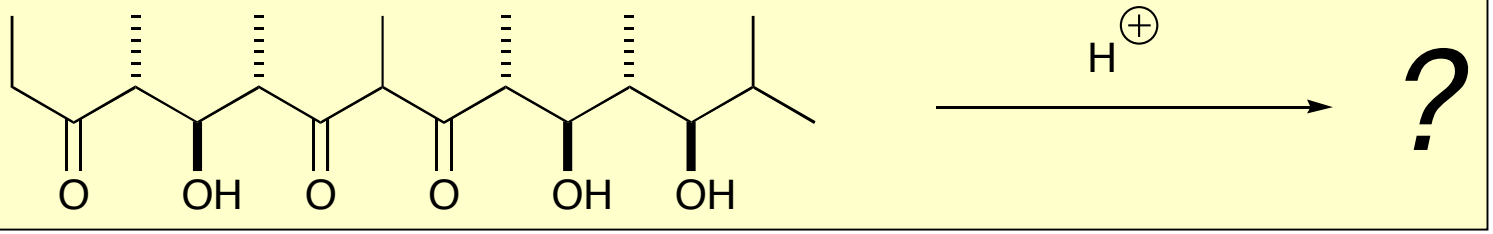
J. E. Davies, I. Fleming and J. M. Goodman *Organic and Biomolecular Chemistry* 2003, **1**, 3570-3571.

No time



preservative vitamin C poison

Similar molecules do different things



Reaction InChI *(RInChI)*

1) Is it possible to extend InChIs to reactions…
2) …and do something useful…
3) …that no one else is doing…
4) …and make it easy to use…
5) …and get people to use it…
6) …?????

A Reaction Identifier ?
issues

- Reactions make molecules seem easy
- Reaction space is much bigger than chemical space
- CAS, Beilstein *et al.* provide excellent resources
- Electronic Lab Notebooks (ELNs) make this obsolete
- Chemistry is too hard to communicate to toxicologists, nano-scientists, biologists, *etc*

A Reaction Identifier ? *possibilities*

- Could different people working on the same reaction could produce the same identifier without communicating?
- Find duplication without sharing data (InChIKey)
- Could different reaction lists be combined easily?
- CAS, Beilstein *et al.* are not open and are slow to be updated
- How are Electronic Lab Notebooks going?
- Toxicologists, nano-scientists, biologists, *etc*, need chemistry (both molecules and reactions)

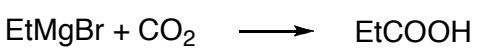
Extend InChI to reactions?

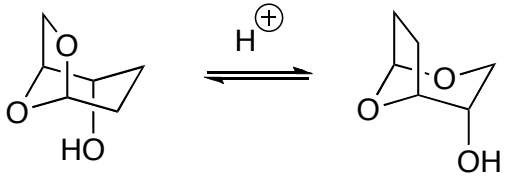
- “The IUPAC International Chemical Identifier (InChITM) is a non-proprietary identifier for chemical substances that can be used in printed and electronic data sources thus enabling easier linking of diverse data compilations”

Extend InChI to reactions?

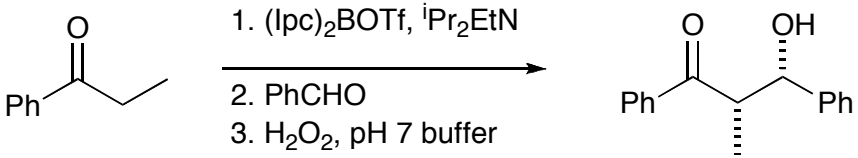
- The Royal Society of Chemistry has sponsored summer students
- IUPAC is sponsoring Reaction InChIs
- Undergraduate Student Projects

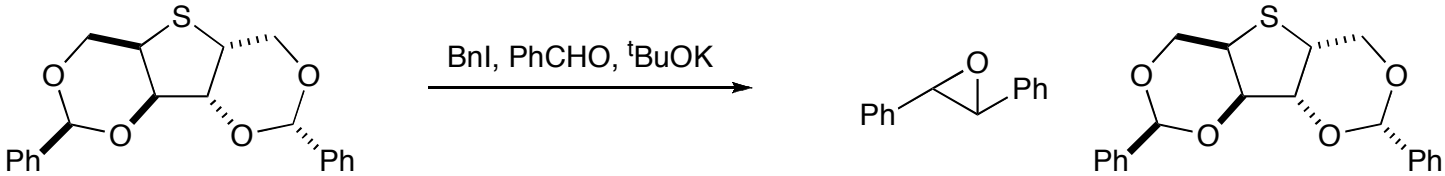
Reactions are hard to describe

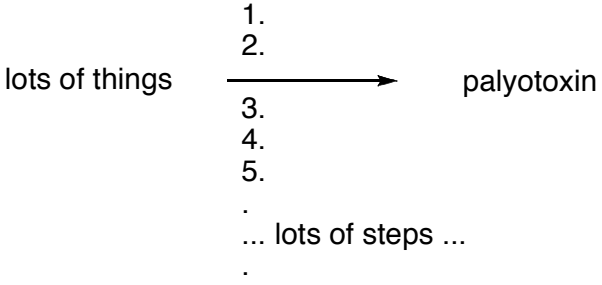
A 

B 

What should be included?
What should be omitted?

C 

D 

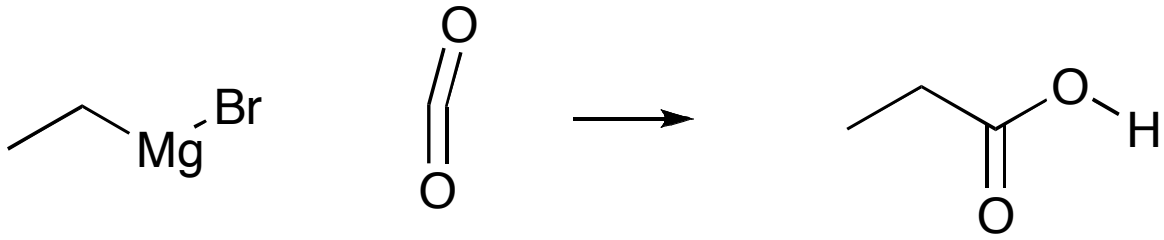
E 

RInChI version 0.1

```
RInChI = version #
  / LHS InChI 1 // LHS InChI 2 ...
  /// RHS InChI 1 // LHS InChI 2
  ...
  /// both sides InChI 1 // both
  sides InChI 2 ...
  /// additional information
```

RInChI version 0.01

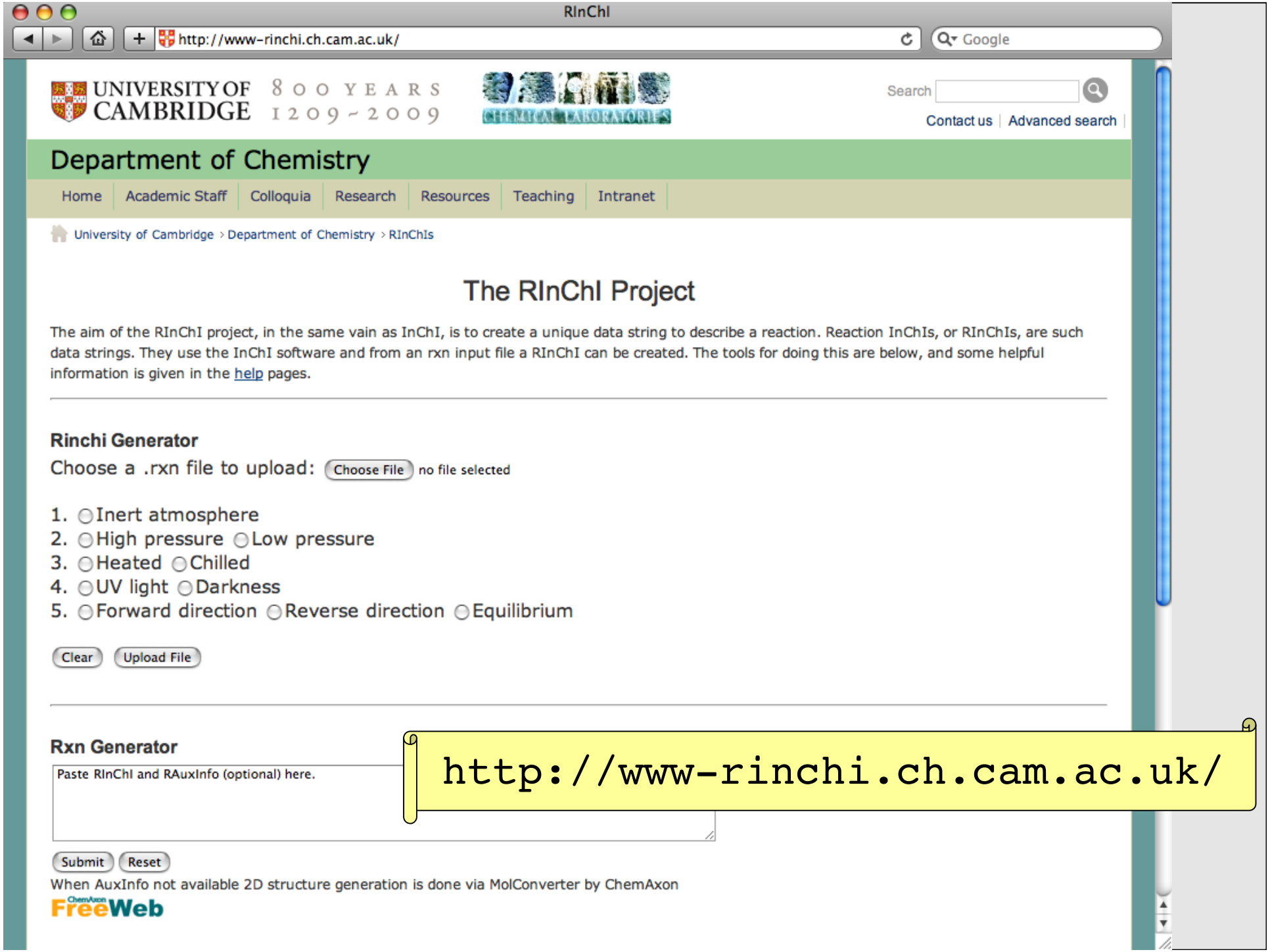
RInChI=0.01.1S/C2H5.BrH.Mg/c1-2;;/h1H2,2H3;1H;/q;;+1/p-1//CO2/c2-1-3///C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5)/d+



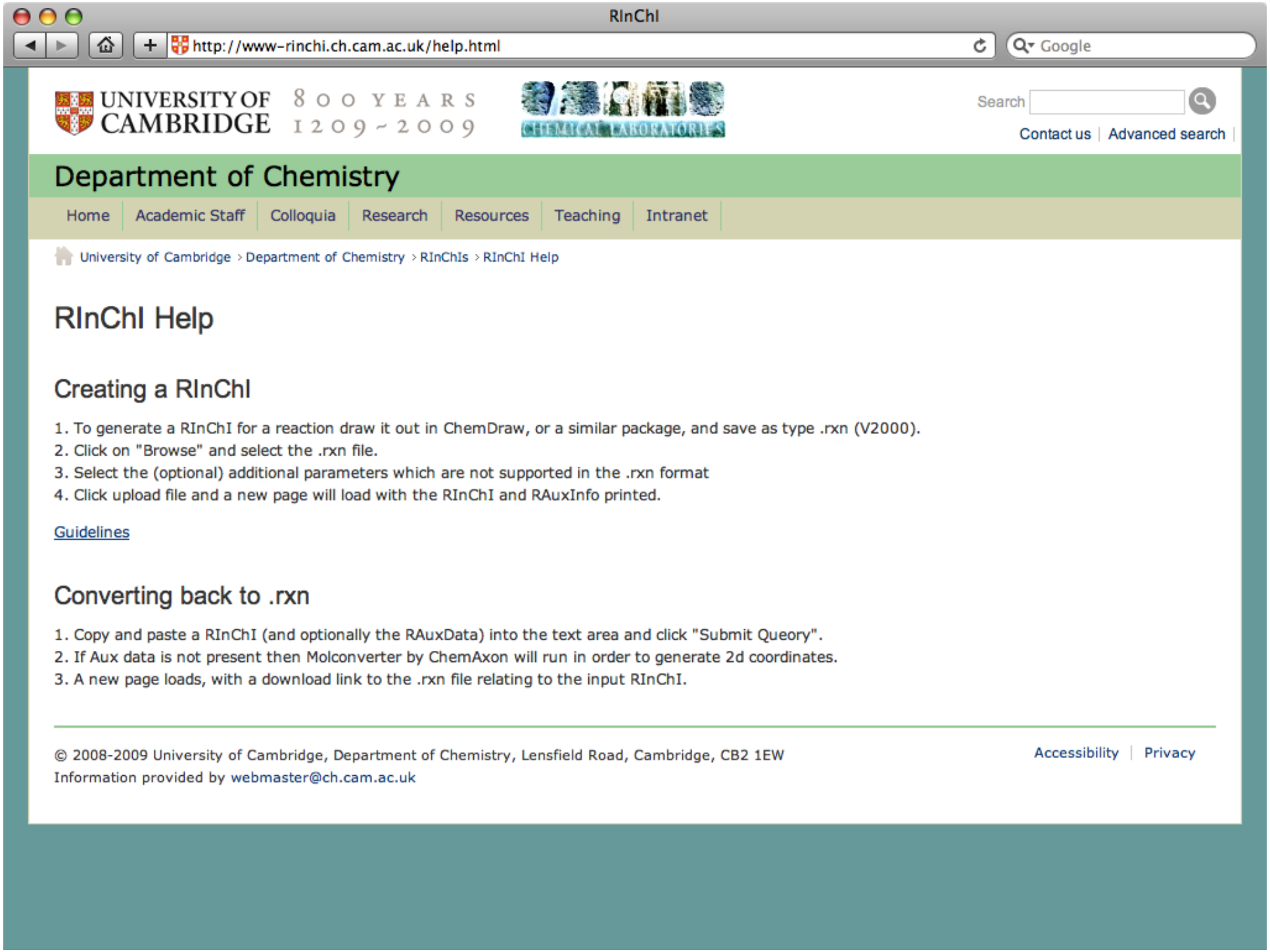
RInChI= version (RinChI.InChI)

/ reactants: InChI#1 // InChI#2

/// product: InChI#1 / reaction direction


RInChI
http://www-rinchi.ch.cam.ac.uk/
Google
UNIVERSITY OF CAMBRIDGE
800 YEARS 1209-2009
CHEMICAL LABORATORIES
Search
Contact us | Advanced search
Department of Chemistry
Home
Academic Staff
Colloquia
Research
Resources
Teaching
Intranet
University of Cambridge › Department of Chemistry › RInChIs
The RInChI Project
The aim of the RInChI project, in the same vain as InChI, is to create a unique data string to describe a reaction. Reaction InChIs, or RInChIs, are such data strings. They use the InChI software and from an rxn input file a RInChI can be created. The tools for doing this are below, and some helpful information is given in the help pages.
Rinchi Generator
Choose a .rxn file to upload:
Choose File
no file selected
1. Inert atmosphere
2. High pressure Low pressure
3. Heated Chilled
4. UV light Darkness
5. Forward direction Reverse direction Equilibrium
Clear
Upload File
Rxn Generator
Paste RInChI and RAuxInfo (optional) here.
Submit
Reset
When AuxInfo not available 2D structure generation is done via MolConverter by ChemAxon
FreeWeb
http://www-rinchi.ch.cam.ac.uk/

RInChI=0.01.1S/2C2H4O2.Hg/c2*1-2(3)4;/h2*1H3,(H,3,4);/q;;+2/p-2//C4H6/c1-3-4-2/h1H,4H2,2H3//H2O/h1H2///C4H8O/c1-3-4(2)5/h3H2,1-2H3///p+1
RInChI=0.01.1S/2C2H4O2.Hg/c2*1-2(3)4;/h2*1H3,(H,3,4);/q;;+2/p-2//BH4.Na/h1H4;/q-1;+1//C4H6/c1-3-4-2/h1H,4H2,2H3//H2O/h1H2///C4H10O/c1-3-4(2)5/h4-5H,3H2,1-2H3///p+1
RInChI=0.01.1S/4O.Os//C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+///C6H14O2/c1-4-6(3,8)5(2)7/h5,7-8H,4H2,1-3H3/t5-,6-/m0/s1
RInChI=0.01.1S/Al.Li.4H/q-1;+1;;;;//C6H10O/c1-3-5-6(7)4-2/h6-7H,4H2,1-2H3///C6H12O/c1-3-5-6(7)4-2/h3,5-7H,4H2,1-2H3/b5-3+
RInChI=0.01.1S/BH2.Na/h1H2;/q+1;-1//C8H14O/c1-6(2)5-8(9)7(3)4/h5,7H,1-4H3//C8H18O3/c1-5-9-8(4,10-6-2)11-7-3/h5-7H2,1-4H3//p+1///C12H22O2/c1-6-14-11(13)9-12(4,5)8-7-
10(2)3/h7-8,10H,6,9H2,1-5H3/b8-7+
RInChI=0.01.1S/BH3/h1H3//C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+///C6H15B/c1-4-5(2)6(3)7/h5-6H,4,7H2,1-3H3/t5-,6+/m1/s1
RInChI=0.01.1S/BH4/h1H4/q-1//C10H12O/c1-8(9(2)11)10-6-4-3-5-7-10/h3-8H,1-2H3/t8-/m1/s1//Na/q+1///C10H14O/c1-8(9(2)11)10-6-4-3-5-7-10/h3-9,11H,1-2H3/t8-
,9+/m1/s1//C10H14O/c1-8(9(2)11)10-6-4-3-5-7-10/h3-9,11H,1-2H3/t8-,9-/m1/s1
RInChI=0.01.1S/BH4/h1H4/q-1//C6H15N/c1-4-7(5-2)6-3/h4-6H2,1-3H3//C8H14O2/c1-5-6(2)8(10)3-7(5)4-9/h5-7,9H,3-4H2,1-2H3/t5-,6-,7+/m1/s1//CH3ClO2S/c1-
5(2,3)4/h1H3//H3N/h1H3//Na/q+1///C8H15N/c1-5-6(2)8-3-7(5)4-9-8/h5-9H,3-4H2,1-2H3/t5-,6-,7?,8?/m1/s1
RInChI=0.01.1S/Br2/c1-2//C3H7NO/c1-2-3(4)5/h2H2,1H3,(H2,4,5)//Na.H2O/h;1H2/q+1;/p-1///C2H7N/c1-2-3/h2-3H2,1H3
RInChI=0.01.1S/Br2/c1-2//C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3+///C4H8Br2/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4+
RInChI=0.01.1S/Br2/c1-2//C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3+//H2O/h1H2///C4H9BrO/c1-3(5)4(2)6/h3-4,6H,1-2H3/t3-,4+/m1/s1
RInChI=0.01.1S/Br2/c1-2//C5H8/c1-3-5-4-2/h3H2,1-2H3///C5H8Br2/c1-3-5(7)4(2)6/h3H2,1-2H3/b5-4+
RInChI=0.01.1S/Br2/c1-2//C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+/i4D///C6H12Br2/c1-4-6(3,8)5(2)7/h5H,4H2,1-3H3/t5-,6+/m1/s1/i5D
RInChI=0.01.1S/Br2/c1-2//C9H8/c1-2-6-9-7-4-3-5-8-9/h3-5,7-8H,1H3///C9H8Br2/c1-7(10)9(11)8-5-3-2-4-6-8/h2-6H,1H3
RInChI=0.01.1S/BrH/h1H//C2H4/c1-2/h1-2H2///C2H5Br/c1-2-3/h2H2,1H3
RInChI=0.01.1S/BrH/h1H//C3H6/c1-3-2/h3H,1H2,2H3///C3H7Br/c1-3(2)4/h3H,1-2H3
RInChI=0.01.1S/BrH/h1H//C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+/i4D///C6H13Br/c1-4-6(3,7)5-2/h4-5H2,1-3H3/i4D/t4-,6?/m0/s1
RInChI=0.01.1S/C11H14FNO/c1-3-13(4-2)11(14)9-6-5-7-10(12)8-9/h5-8H,3-4H2,1-2H3//C4H9.Li/c1-3-4-2;/h1,3-4H2,2H3;//C7H6O/c8-6-7-4-2-1-3-5-7/h1-6H///C18H20FNO2/c1-3-20(4-
2)18(22)14-11-8-12-15(19)16(14)17(21)13-9-6-5-7-10-13/h5-12,17,21H,3-4H2,1-2H3/t17-/m0/s1
RInChI=0.01.1S/C12H14O2/c1-8(2)11-10(12(13)14-11)9-6-4-3-5-7-9/h3-8,10-11H,1-2H3//C6H14N/c1-5(2)7-6(3)4/h5-6H,1-4H3/q-1//C7H7Br/c8-6-7-4-2-1-3-5-7/h1-
5H,6H2//Li/q+1///C19H20O2/c1-14(2)17-19(18(20)21-17,16-11-7-4-8-12-16)13-15-9-5-3-6-10-15/h3-12,14,17H,13H2,1-2H3/t17-,19+/m1/s1
RInChI=0.01.1S/C12H22BCl/c14-13(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h11-12H,1-10H2//C6H15N/c1-4-7(5-2)6-3/h4-6H2,1-3H3//C7H6O/c8-6-7-4-2-1-3-5-7/h1-6H//C9H16O/c1-2-9(10)8-
6-4-3-5-7-8/h8H,2-7H2,1H3///C16H22O2/c1-12(15(17)13-8-4-2-5-9-13)16(18)14-10-6-3-7-11-14/h2,4-5,8-9,12,14-15,17H,3,6-7,10-11H2,1H3/t12-,15+/m1/s1
RInChI=0.01.1S/C16H24O5SSi/c1-11-15(23(4,5)13-9-7-6-8-10-13)14(20-16(11)17)12(2)21-22(3,18)19/h6-12,14-15H,1-5H3/t11-,12+,14?,15+/m0/s1//N3/c1-3-2/q-
1///C15H21N3O2Si/c1-10-14(13(20-15(10)19)11(2)17-18-16)21(3,4)12-8-6-5-7-9-12/h5-11,13-14H,1-4H3/t10-,11-,13?,14+/m0/s1
RInChI=0.01.1S/C18H15P/c1-4-10-16(11-5-1)19(17-12-6-2-7-13-17)18-14-8-3-9-15-18/h1-15H//C2H6O/c1-2-3/h3H,2H2,1H3//CCl4/c2-1(3,4)5///C2H5Cl/c1-2-3/h2H2,1H3
RInChI=0.01.1S/C21H34BF3O3S/c1-11-15-7-13(19(15,3)4)9-17(11)22(28-29(26,27)21(23,24)25)18-10-14-8-16(12(18)2)20(14,5)6/h11-18H,7-10H2,1-6H3//C7H6O/c8-6-7-4-2-1-3-5-
7/h1-6H//C8H19N/c1-6-9(7(2)3)8(4)5/h7-8H,6H2,1-5H3//C9H10O/c1-2-9(10)8-6-4-3-5-7-8/h3-7H,2H2,1H3//H2O2/c1-2/h1-2H///C16H16O2.CH4/c1-12(15(17)13-8-4-2-5-9-13)16(18)14-
10-6-3-7-11-14;/h2-12,15,17H,1H3;1H4
RInChI=0.01.1S/C2H2/c1-2/h1-2H//CO2/c2-1-3//H2N.Na/h1H2;/q-1;+1///C3H2O2/c1-2-3(4)5/h1H,(H,4,5)/p-1
RInChI=0.01.1S/C2H4O3/c1-2(3)5-4/h4H,1H3//C5H8/c1-2-4-5-3-1/h1-2H,3-5H2///C5H8O/c1-2-4-5(3-1)6-4/h4-5H,1-3H2
RInChI=0.01.1S/C2H4O3/c1-2(3)5-4/h4H,1H3//C5H8O/c6-5-3-1-2-4-5/h1-4H2///C5H8O2/c6-5-3-1-2-4-7-5/h1-4H2
RInChI=0.01.1S/C2H5.BrH.Mg/c1-2;;/h1H2,2H3;1H;/q;;+1/p-1//CO2/c2-1-3///C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5)
RInChI=0.01.1S/C2H6S.BrH.Cu/c1-3-2;;/h1-2H3;1H;/q;;+1/p-1//C4H7.BrH.Mg/c1-3-4-2;;/h3H,1-2,4H2;1H;/q;;+1/p-1//C8H8O3/c1-8-3-2-5(9)6(4-8)11-7(8)10/h2-3,6H,4H2,1H3/t6-,8-
/m0/s1///C12H16O3/c1-3-4-5-8-6-9(13)10-7-12(8,2)11(14)15-10/h3,8,10H,1,4-7H2,2H3/t8-,10+,12-/m1/s1
RInChI=0.01.1S/C2H6S/c1-3-2/h1-2H3//C6H12/c1-3-5-6-4-2/h5-6H,3-4H2,1-2H3/b6-5+//C6H14N/c1-5(2)7-6(3)4/h5-6H,1-4H3/q-1//Li/q+1///C2H4O/c1-2-3/h2H,1H3
RInChI=0.01.1S/C3H6O/c1-3(2)4/h1-2H3///C6H10O/c1-5(2)4-6(3)7/h4H,1-3H3//p+1
RInChI=0.01.1S/C4H10O/c1-4(2,3)5/h5H,1-3H3//C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3+//C5H11NO2/c1-6(7)2-4-8-5-3-6/h2-5H2,1H3//H2O/h1H2///C4H10O2/c1-3(5)4(2)6/h3-6H,1-2H3///4O.Os
RInChI=0.01.1S/C4H10O/c1-4(2,3)5/h5H,1-3H3//C5H8/c1-3-5-4-2/h3H2,1-2H3//Na.H///C4H9O/c1-4(2,3)5/h1-3H3/q-1//C5H10/c1-3-5-4-2/h3,5H,4H2,1-2H3/b5-3+///H3N/h1H3
RInChI=0.01.1S/C4H2/c1-3-4-2/h1-2H//CH3O/c1-2/h1H3/q-1//CH4O/c1-2/h2H,1H3///C5H6O/c1-3-4-5-6-2/h1,4-5H,2H3/b5-4-
RInChI=0.01.1S/C4H7Br/c1-2-3-4-5/h2-3H,4H2,1H3//C4H9.Li/c1-3-4-2;/h1,3-4H2,2H3;//C7H5ClO/c8-7(9)6-4-2-1-3-5-6/h1-5H///C15H19NO/c1-4-5-8-12-9-6-7-10-13(12)14-16-
15(2,3)11-17-14/h4-7,9-10H,8,11H2,1-3H3
RInChI=0.01.1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3/t3-,4?/m0/s1//CH3.BrH.Mg/h1H3;1H;/q;;+1/p-1//ClH.Cu/h1H;/q;+1/p-1///C5H12O/c1-4(2)5(3)6/h4-6H,1-3H3
RInChI=0.01.1S/C4H9BrO/c1-3(5)4(2)6/h3-4,6H,1-2H3/t3-,4+/m1/s1//Na.H2O/h;1H2/q+1;/p-1///C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3/t3-,4?/m0/s1
RInChI=0.01.1S/C4H9NO/c1-3-4(2)5-6/h6H,3H2,1-2H3/b5-4+//p+1///C4H9NO/c1-3-5-4(2)6/h3H2,1-2H3,(H,5,6)
RInChI=0.01.1S/C4H9O.K/c1-4(2,3)5;/h1-3H3;/q-1;+1//C7H13Cl/c1-7(8)5-3-2-4-6-7/h2-6H2,1H3///C7H12/c1-7-5-3-2-4-6-7/h1-6H2
RInChI=0.01.1S/C4H9O/c1-4(2,3)5/h1-3H3/q-1//C7H6O/c8-6-7-4-2-1-3-5-7/h1-6H//C7H7I/c8-6-7-4-2-1-3-5-7/h1-5H,6H2//K/q+1///C14H12O/c1-3-7-11(8-4-1)13-14(15-13)12-9-5-2-6-
10-12/h1-10,13-14H/t13-,14-/m1/s1///C20H20O4S/c1-3-7-13(8-4-1)19-21-11-15-17(23-19)18-16(25-15)12-22-20(24-18)14-9-5-2-6-10-14/h1-10,15-20H,11-12H2/t15-,16-
,17+,18?,19+,20+/m1/s1
RInChI=0.01.1S/C5H10O2/c1-3-5(6)7-4-2/h3-4H2,1-2H3//CH3O.Na/c1-2;/h1H3;/q-1;+1//p+1///C8H14O3/c1-4-7(9)6(3)8(10)11-5-2/h6H,4-5H2,1-3H3
RInChI=0.01.1S/C5H8/c1-3-5-4-2/h3H2,1-2H3//H2/h1H///C5H10/c1-3-5-4-2/h3,5H,4H2,1-2H3/b5-3-
RInChI=0.01.1S/C6H10O/c7-6-4-2-1-3-5-6/h2,4,6-7H,1,3,5H2//C7H5ClO3/c8-6-3-1-2-5(4-6)7(9)11-10/h1-4,10H///C8H12O3/c1-5(9)10-6-3-2-4-7-8(6)11-7/h6-8H,2-4H2,1H3/t6-
,7?,8?/m1/s1
RInChI=0.01.1S/C6H10O3/c7-4-1-2-6-8-3-5(4)9-6/h4-7H,1-3H2///C6H10O3/c7-4-3-8-6-2-1-5(4)9-6/h4-7H,1-3H2///p+1
RInChI=0.01.1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+//C7H5ClO3/c8-6-3-1-2-5(4-6)7(9)11-10/h1-4,10H///C6H12O/c1-4-6(3)5(2)7-6/h5H,4H2,1-3H3/t5-,6-/m0/s1
RInChI=0.01.1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3/b6-4+//H2O/h1H2///C6H14O/c1-4-6(3,7)5-2/h7H,4-5H2,1-3H3///p+1
RInChI=0.01.1S/C6H12O/c1-4-6(3)5(2)7-6/h5H,4H2,1-3H3/t5-,6-/m0/s1//H2O/h1H2/p-1///C6H14O2/c1-4-6(3,8)5(2)7/h5,7-8H,4H2,1-3H3/t5-,6+/m1/s1
RInChI=0.01.1S/C6H15B/c1-4-5(2)6(3)7/h5-6H,4,7H2,1-3H3/t5-,6+/m1/s1//H2O/h1H2/p-1//H2O2/c1-2/h1-2H///C6H14O/c1-4-5(2)6(3)7/h5-7H,4H2,1-3H3/t5-,6+/m1/s1
RInChI=0.01.1S/C6H5Br/c7-6-4-2-1-3-5-6/h1-5H//H2N.Na/h1H2;/q-1;+1///C6H7N/c7-6-4-2-1-3-5-6/h1-5H,7H2
RInChI=0.01.1S/C7H14O/c1-7(8)5-3-2-4-6-7/h8H,2-6H2,1H3///C7H12/c1-7-5-3-2-4-6-7/h5H,2-4,6H2,1H3///p+1
RInChI=0.01.1S/C7H5ClO3/c8-6-3-1-2-5(4-6)7(9)11-10/h1-4,10H//C8H12O2/c1-7(9)10-8-5-3-2-4-6-8/h3,5,8H,2,4,6H2,1H3///C8H12O3/c1-5(9)10-6-3-2-4-7-8(6)11-7/h6-8H,2-
4H2,1H3/t6-,7?,8?/m1/s1


RInChI
http://www-rinchi.ch.cam.ac.uk/help.html
Google
UNIVERSITY OF CAMBRIDGE
800 YEARS 1209-2009
CHEMICAL LABORATORIES
Search
Contact us | Advanced search
Department of Chemistry
Home | Academic Staff | Colloquia | Research | Resources | Teaching | Intranet
University of Cambridge › Department of Chemistry › RInChIs › RInChI Help
RInChI Help
Creating a RInChI
1. To generate a RInChI for a reaction draw it out in ChemDraw, or a similar package, and save as type .rxn (V2000).
2. Click on "Browse" and select the .rxn file.
3. Select the (optional) additional parameters which are not supported in the .rxn format
4. Click upload file and a new page will load with the RInChI and RAuxInfo printed.
Guidelines
Converting back to .rxn
1. Copy and paste a RInChI (and optionally the RAuxData) into the text area and click "Submit Queory".
2. If Aux data is not present then Molconverter by ChemAxon will run in order to generate 2d coordinates.
3. A new page loads, with a download link to the .rxn file relating to the input RInChI.
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RInChI Guidelines

To help ensure a reaction generates the same RInChI for every person there are some rules which must be followed with regard what to include and where:

1. Specify all reactants on the left hand side, including solvents and catalysts.
2. Specify main products on the right hand side, as well as solvents and catalysts.
3. For a reactions involving multiple step, specify all reactants on the left side, including solvents and catalysts. On the right side specify only the main products and the solvents and catalysts present in the last step of the reaction.
4. Acids and bases may be specified by H+ and OH- to be more general.

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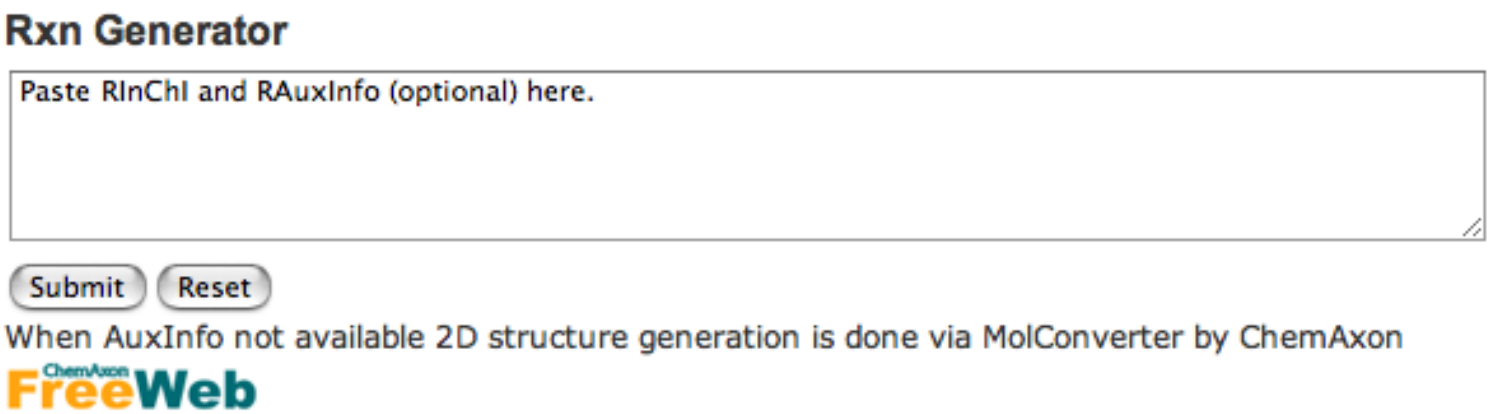
Accessibility

Reading, Writing and Arithmetic



RInChI can be converted into .rxn files.

2D geometries may be in the Auxiliary Information, or else generated by ChemAxon's MolConverter

Reading, **Writing** and Arithmetic

1. ○ Inert atmosphere
2. ○ High pressure ○ Low pressure
3. ○ Heated ○ Chilled
4. ○ UV light ○ Darkness
5. ◉ Forward direction ○ Reverse direction ○ Equilibrium

RInChI are generated from .rxn files.

Some additional information is added as extra layers

Too much information is bad

- different RInChI for closely related processes

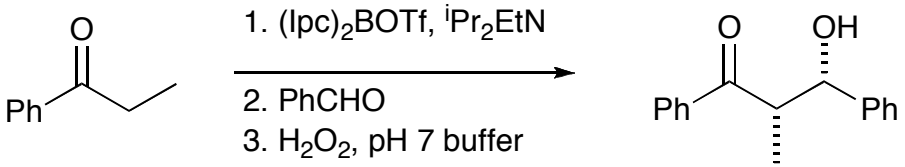
How much is too much? Is this list the right list?

Reading, Writing and **Arithmetic**

Rinchi Addition

Paste RInChIs (and RAuxInfo) here. Do not include additional information.
eg:
RInChI 1
(RAuxInfo 1)
RInChI 2

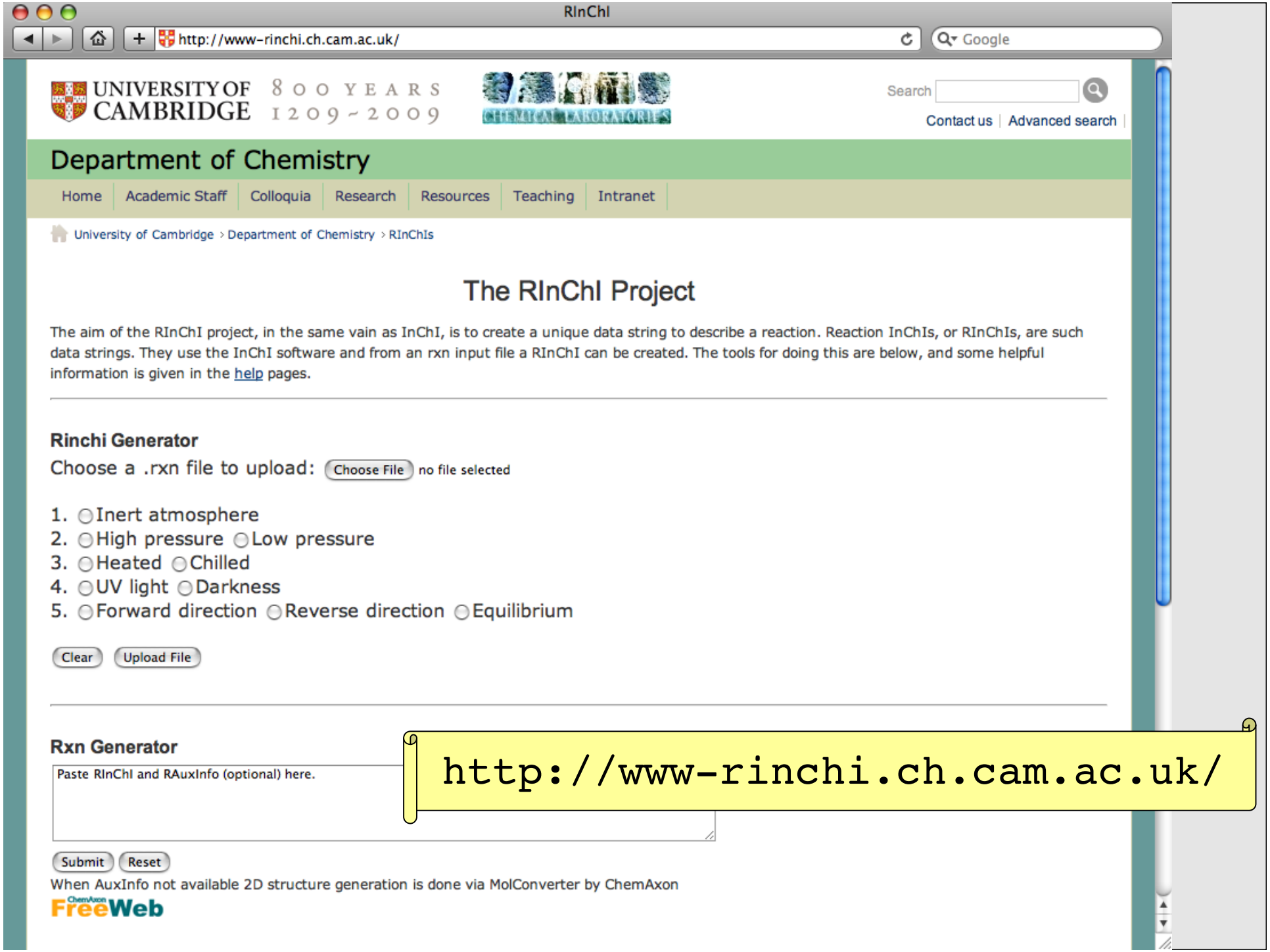
Submit Reset



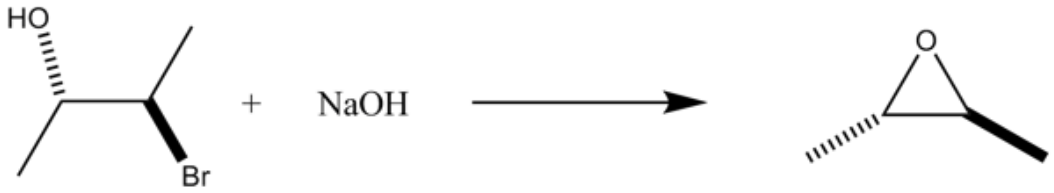
One RInChI or Three RInChI ?

The three separate RInChIs for each step can be added up to form a single RInChI for the whole process.

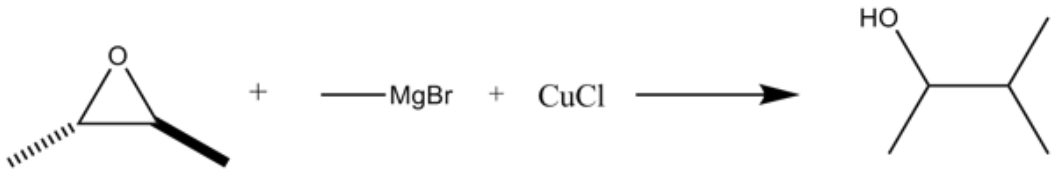
If some authors consider a reaction to be one step, and others the same reaction to be two steps, they should have the same RInChI for the whole transformation


RInChI
http://www-rinchi.ch.cam.ac.uk/
Google
UNIVERSITY OF CAMBRIDGE
800 YEARS 1209-2009
CHEMICAL LABORATORIES
Search
Contact us | Advanced search
Department of Chemistry
Home
Academic Staff
Colloquia
Research
Resources
Teaching
Intranet
University of Cambridge › Department of Chemistry › RInChIs
The RInChI Project
The aim of the RInChI project, in the same vain as InChI, is to create a unique data string to describe a reaction. Reaction InChIs, or RInChIs, are such data strings. They use the InChI software and from an rxn input file a RInChI can be created. The tools for doing this are below, and some helpful information is given in the help pages.
Rinchi Generator
Choose a .rxn file to upload:
Choose File
no file selected
1. Inert atmosphere
2. High pressure Low pressure
3. Heated Chilled
4. UV light Darkness
5. Forward direction Reverse direction Equilibrium
Clear
Upload File
Rxn Generator
Paste RInChI and RAuxInfo (optional) here.
Submit
Reset
When AuxInfo not available 2D structure generation is done via MolConverter by ChemAxon
FreeWeb
http://www-rinchi.ch.cam.ac.uk/

Example RInChIs



RInChI=0.01.1S/C4H9BrO/c1-3(5)4(2)6/h3-4,6H,1-2H3/t3-,4+/m1/s1//Na.H2O/h;1H2/q+1;/p-1///C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3/t3-,4?/m0/s1
RAuxInfo=0.01.1S/0/N:4,1,3,2,6,5/it:im/rA:6nCCCCOBr/rB:s1;s2;s3;N2;P3;/rC:-.825,-.7557,0;-.4125,-.0412,0;.4125,-.0412,0;.825,.6733,0;-.626,.7557,0;.825,-.7557,0;//1/N:1;2/rA:2nNaO/rB:s1;/rC:-.4125,0,0;.4125,0,0;///0/N:4,1,3,2,5/E:(1,2)(3,4)/it:im/rA:5nCCCCO/rB:N1;s2;P3;s2s3;/rC:-1.127,-.5635,0;-.4125,-.151,0;.4125,-.151,0;1.127,-.5635,0;0,.5635,0;



RInChI=0.01.1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3/t3-,4?/m0/s1//CH3.BrH.Mg/h1H3;1H;/q;;+1/p-1//ClH.Cu/h1H;/q;+1/p-1///C5H12O/c1-4(2)5(3)6/h4-6H,1-3H3
RAuxInfo=0.01.1S/0/N:4,1,3,2,5/E:(1,2)(3,4)/it:im/rA:5nCCCCO/rB:N1;s2;P3;s2s3;/rC:-1.127,-.5635,0;-.4125,-.151,0;.4125,-.151,0;1.127,-.5635,0;0,.5635,0;//1/N:1;3;2/CRV:1.3;;/rA:3nCMgBr/rB:s1;s2;/rC:-.6188,-

Testing RInChI

- Lots of reaction information is omitted:
  - Mechanism
  - Temperatures
  - Yields
  - Quantities
- Different people doing the same reaction should generate the same RInChI without consulting each other
  - Not a registration service
  - Can generate a RInChI without knowing much about the reaction
- Barrier to creating RInChIs should be low
- Misleading RInChIs will inevitably be developed

Testing RInChI

- .rdf files from three companies have been translated into RInChIs and combined
  - This only took a few minutes for about 3 000 reactions
- The RInChI files is 3 % of the size of the .rdf files
- Contains much of the useful information
- The file of RInChIs can easily be manipulated with unix commands
  - Files from different companies readily joined together
  - Find duplicates (sort | uniq -c)
  - Same starting materials, different products
  - Same products, different starting materials
  - Product of one reaction is a starting material for another
  - How many different molecules involved?

Testing RInChI

- Current work:
  - Easy questions, without processing InChI
    - What atoms are different in starting materials and products?
    - Has the number of rings changed?
    - Has the number of chiral centres changed?
    - What bonds have changed?
  - Atom mapping
    - How accurate does it have to be?
      Should the scientist be allowed to get it wrong, or should this be left to the computer?
    - Mechanism?
    - Verification
    - Machine learning
  - Substructure searching

RInChI

- Have we made the right decisions?
- Future work:
  - more layers or fewer?
  - Polymers - encode as the polymerisation conditions?
  - Key reactions - encode with minimal atoms and list permitted substitution positions in optional layer
  - Non-molecular reagents (Raney Nickel, pH7 buffer, *etc*). List through controlled vocabulary and database?
  - Automated checking of RInChI validity?

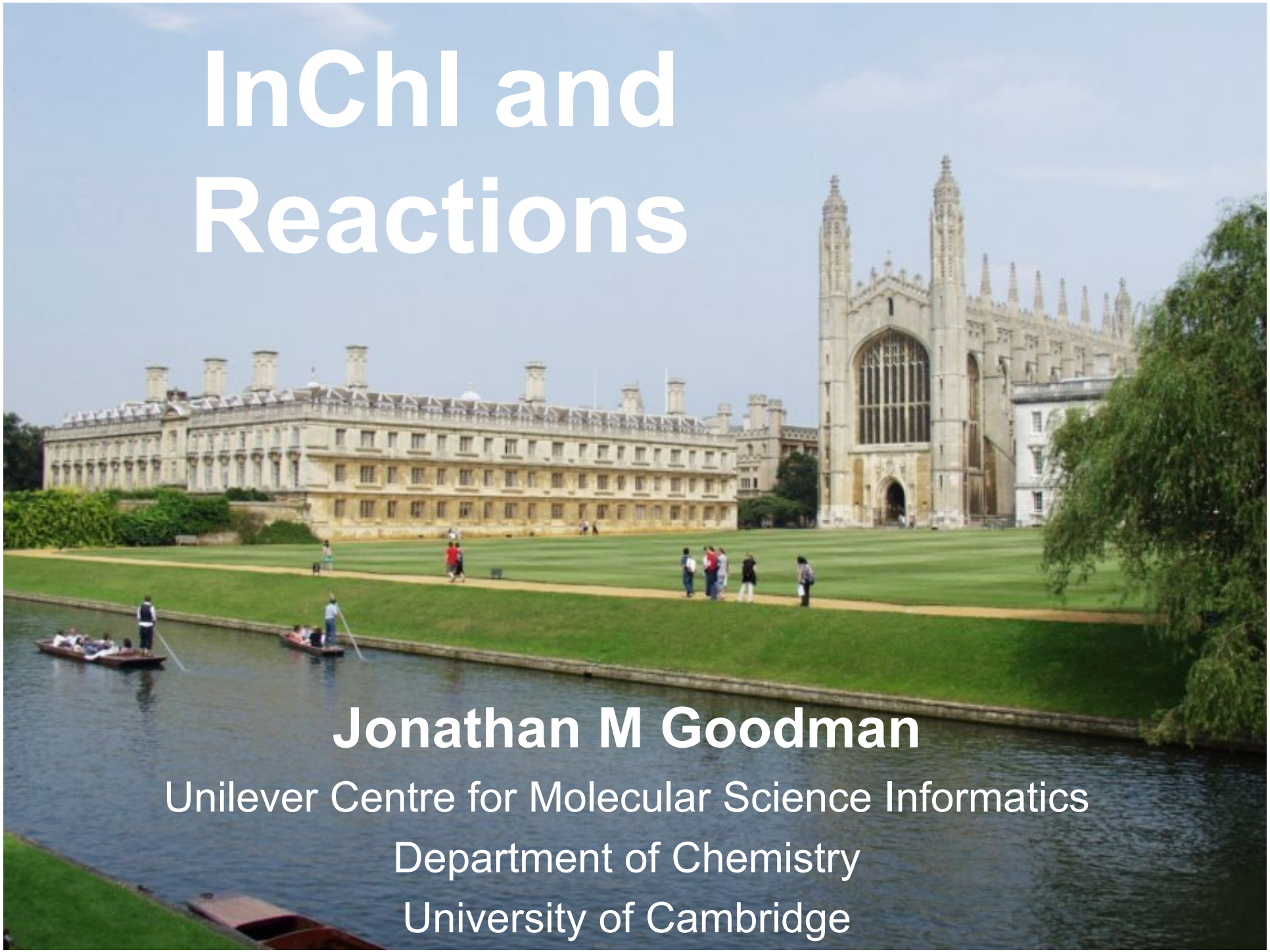
RInChI Summary

- RInChI - *draft version now available*
  - Different groups working independently on one reaction should produce the same RInChI, without communicating
- RInChI:
  - Compact
  - Easy to generate
  - Easy to handle
  - Omits unnecessary information
  - Omits hard-to-find information
  - Omits subjective information
  - Contains the right information
  - Provides a consistent outline of reaction information
  - *A valuable resource for open chemistry*

Reaction InChI *(RInChI)*

1) Is it possible to extend InChIs to reactions…
2) …and do something useful…
3) …that no one else is doing…
4) …and make it easy to use…
5) …and get people to use it…
6) …?????

InChI and Reactions



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Unilever Centre for Molecular Science Informatics

Department of Chemistry

University of Cambridge