Working with

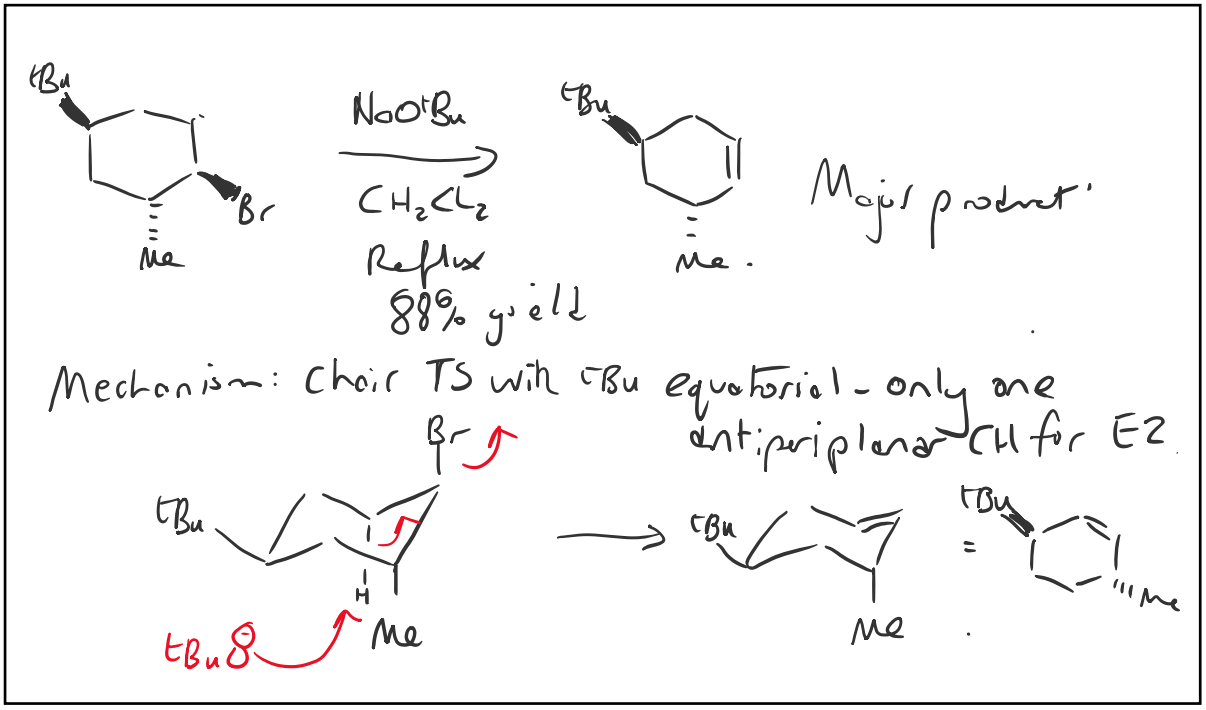
Purpose of this Workshop

- Be able to draw molecules and reactions using Chemdraw
- Understand how to format Chemdraw settings to make structures more aesthetically pleasing
- Know how to embed Chemdraw schemes into MS Office documents (Word/Powerpoint)
- Become a keyboard shortcut ninja

The Challenge

You've performed the following reaction, and you want to

1. Prepare a professional-looking experimental write-up; and
2. Give a discussion of the reaction mechanism.

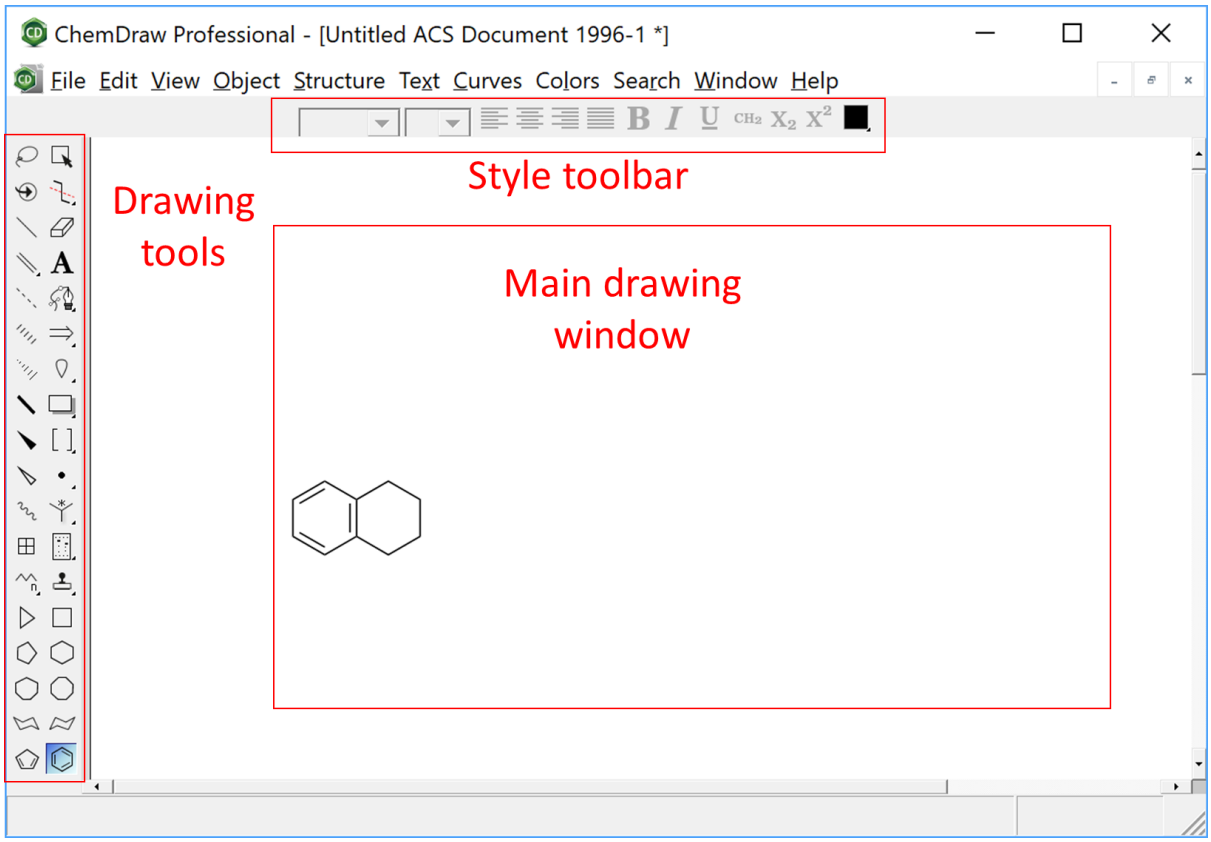


So, you will need to prepare **two chemdraw schemes.**

Getting Started with ChemDraw

This is the main interface for ChemDraw.

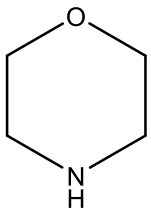
If any toolbars you need are missing, restore them using ***View*** menu.



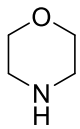
The first thing you should do after installing Chemdraw is to **change the default drawing style**. The quickest way to do this is through ***File>Open Style Sheets>ACS Document*.**

In the future, any new Chemdraw file will default to the ACS document settings, which look much more appealing.

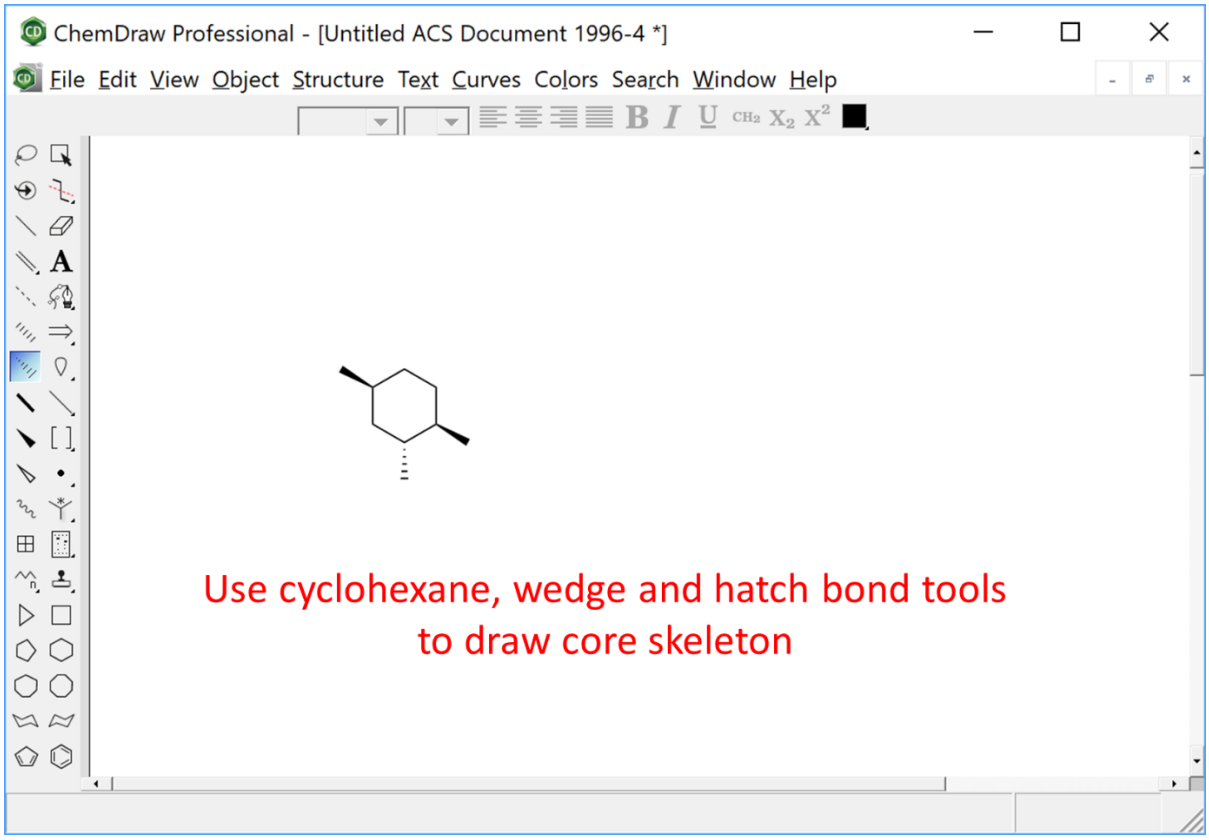
Default style settings

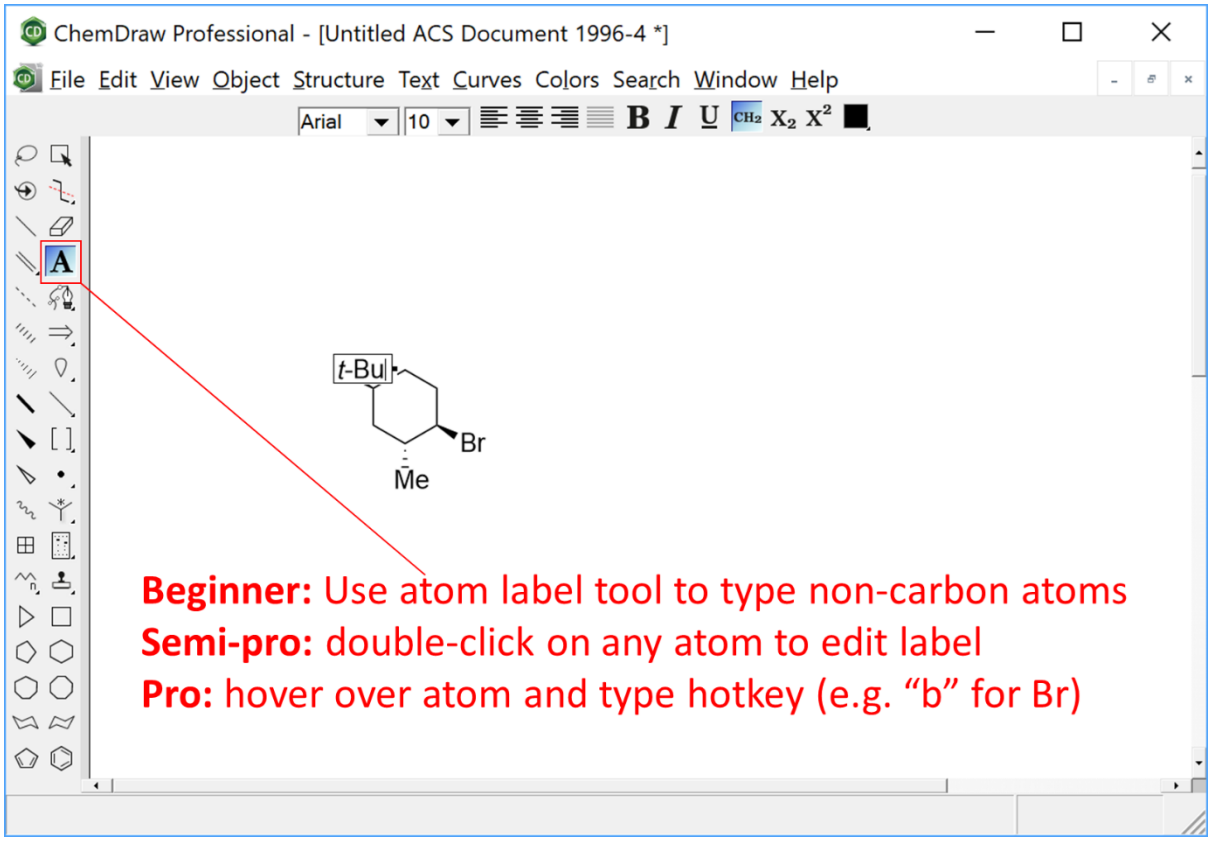


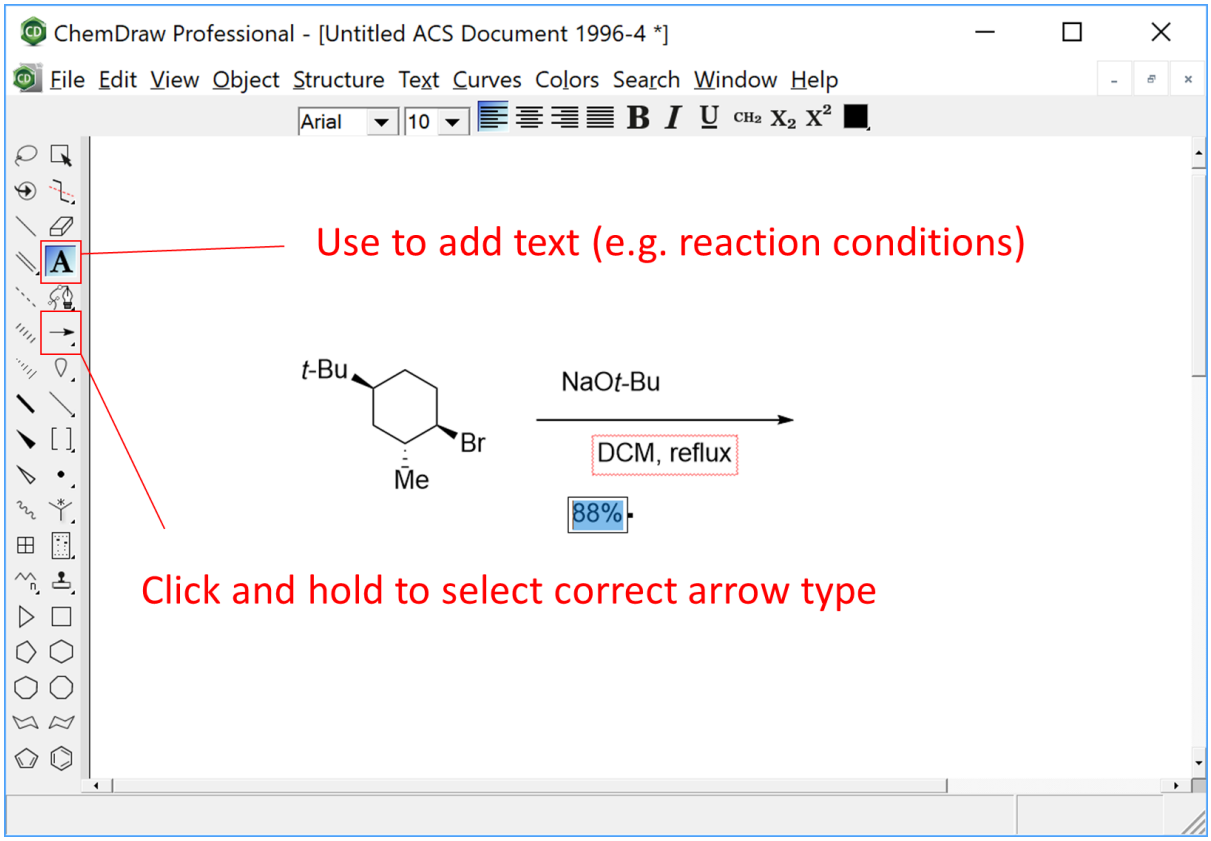
ACS Style Settings

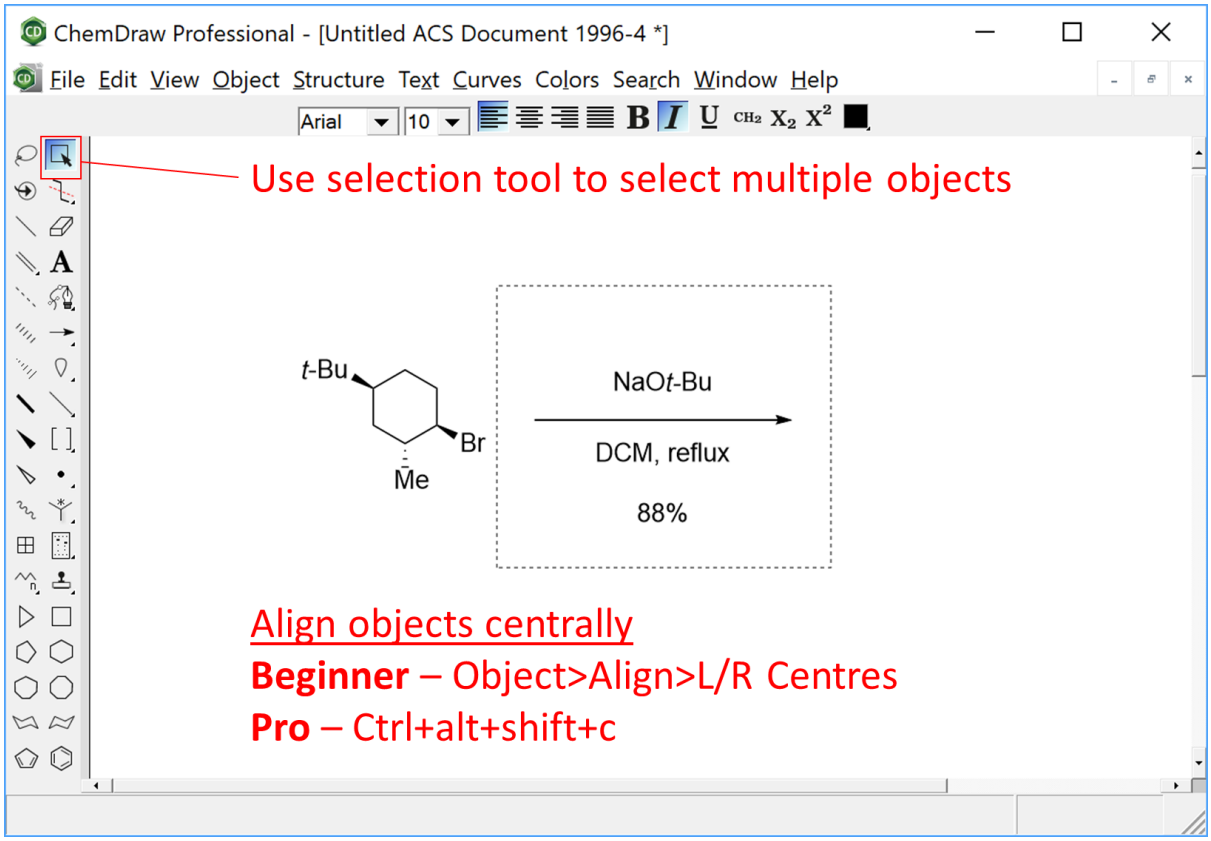


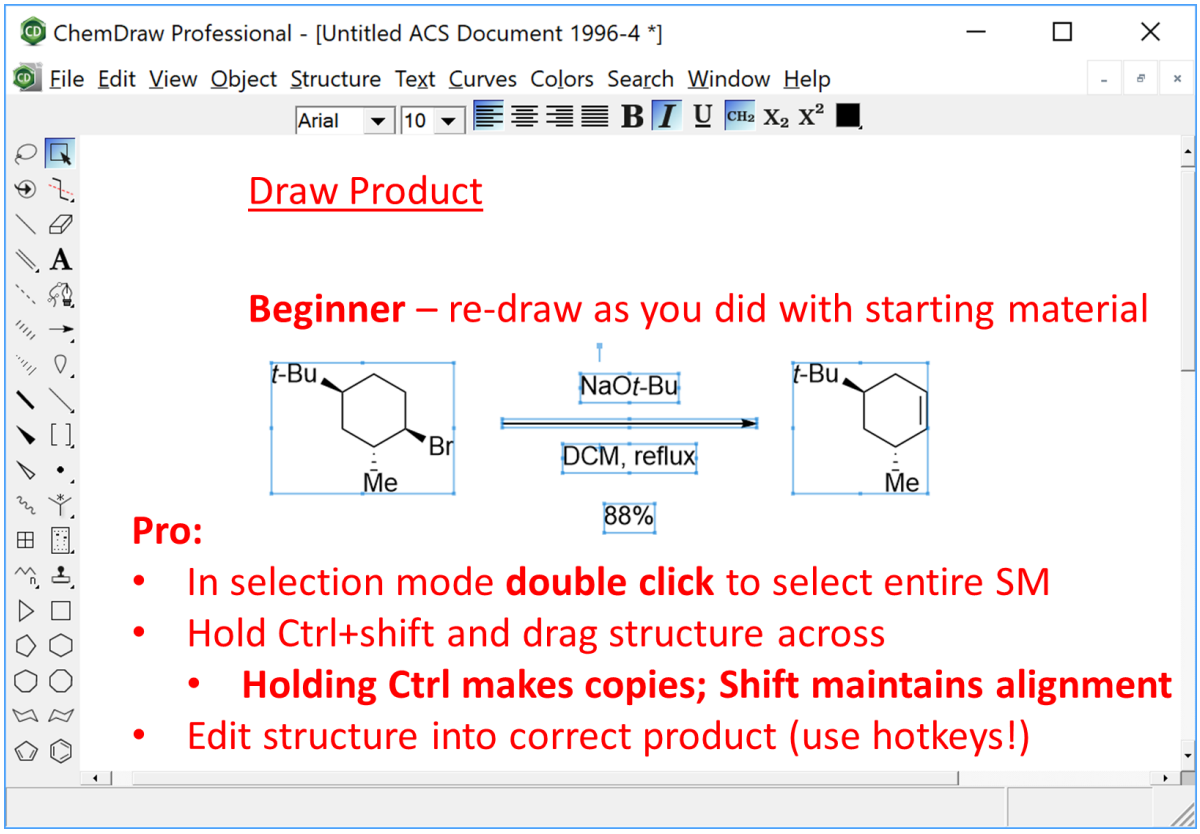
Drawing Your Overall Reaction






ChemDraw Professional - [Untitled ACS Document 1996-4 *]
File Edit View Object Structure Text Curves Colors Search Window Help
Arial 10
Use to add text (e.g. reaction conditions)
t-Bu
Br
Me
NaOt-Bu
DCM, reflux
88%
Click and hold to select correct arrow type

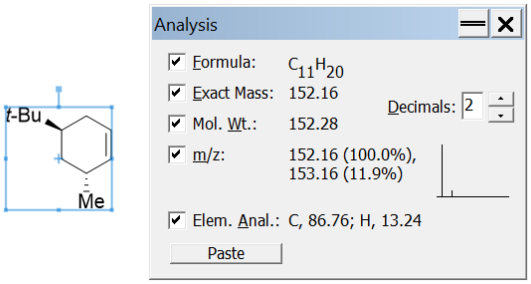

ChemDraw Professional - [Untitled ACS Document 1996-4 *]
File Edit View Object Structure Text Curves Colors Search Window Help
Arial 10
Use selection tool to select multiple objects
t-Bu
Br
Me
NaOt-Bu
DCM, reflux
88%
Align objects centrally
Beginner – Object>Align>L/R Centres
Pro – Ctrl+alt+shift+c



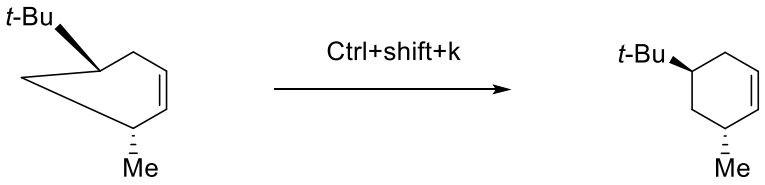
You've just created a professional-looking (unlike this WordArt) Chemdraw scheme.

Other useful functions

- The **Analysis Toolbar** (View>Analysis toolbar) – use to work out molecular weight and formulae:



- The **cleanup tool** (Ctrl+shift+k) – fixes bond angles, lengths etc. Sometimes need to press several times:



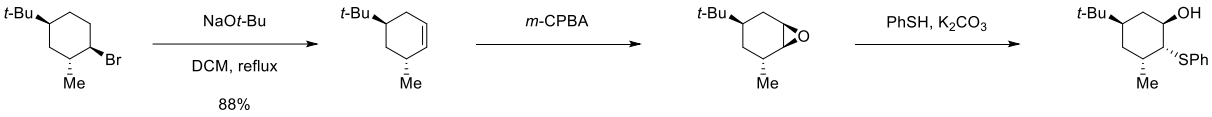
Inserting Chemdraw into MS Office

Office for PCs now makes it extremely simple to work with Chemdraw files. Simple select the items you want, ***copy, and paste into Word or Powerpoint***.

If you want to re-edit these schemes, just double-click on them within Office, and the document will re-open in Chemdraw.

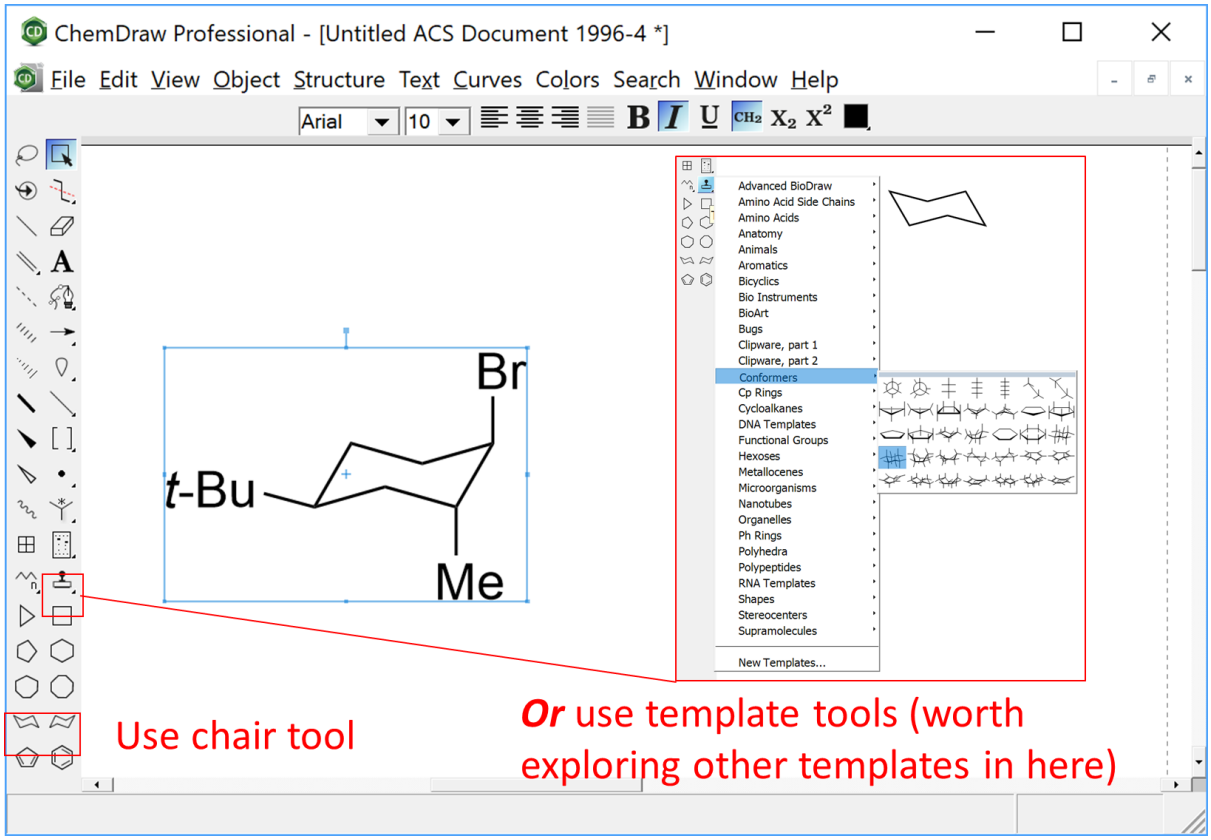
Some cautionary notes:

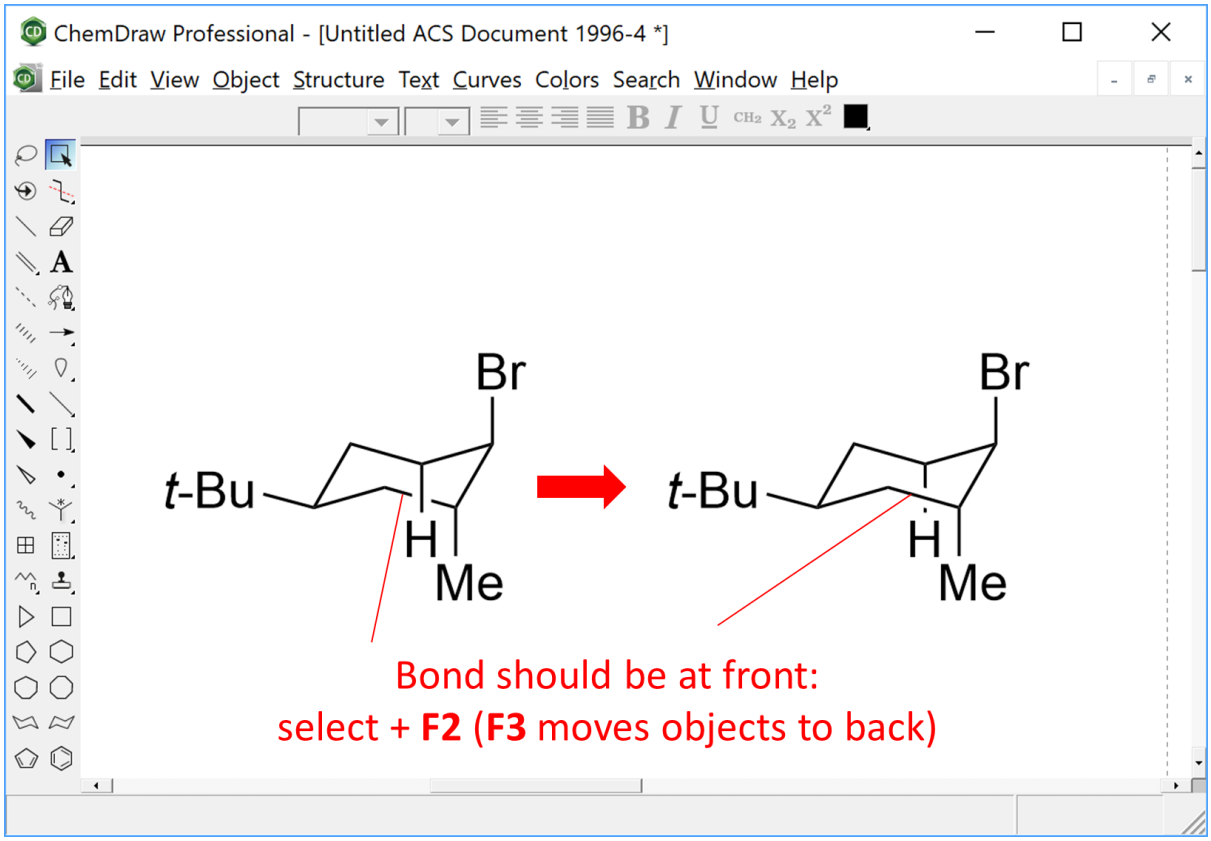
- this so-called “round-trip editing” is currently not supported by Mac OS. Mac users will have to copy Chemdraw schemes out of MS Office and back into Chemdraw to edit them**.**
- It is advisable to separately **save your Chemdraw files**, rather than relying on copies embedded in Word files. Occasionally these become corrupted, and you can no longer edit them. This isn’t a massive problem for a short report, but on a 300 page thesis…
- If your Chemdraw scheme is very wide, Word will automatically shrink it to the width of your page (without telling you), so don’t make overly wide schemes or structures will become tiny, like this:

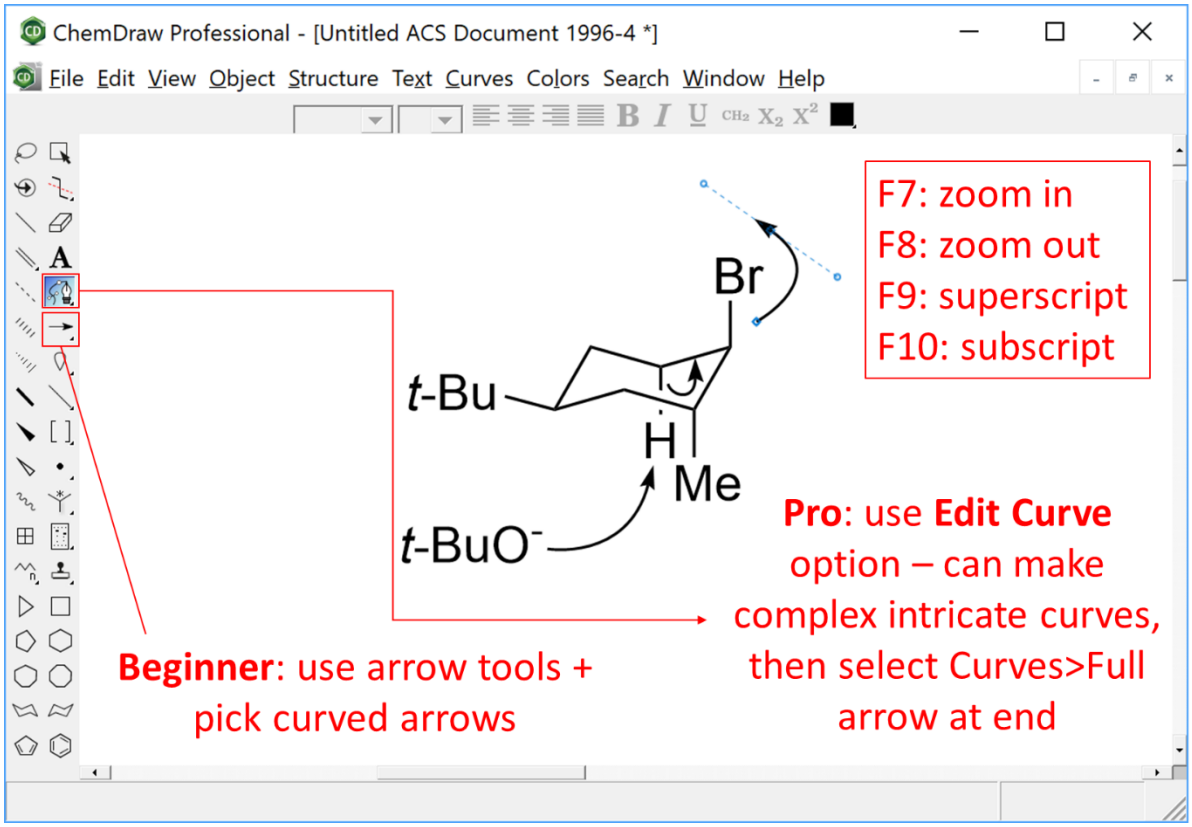


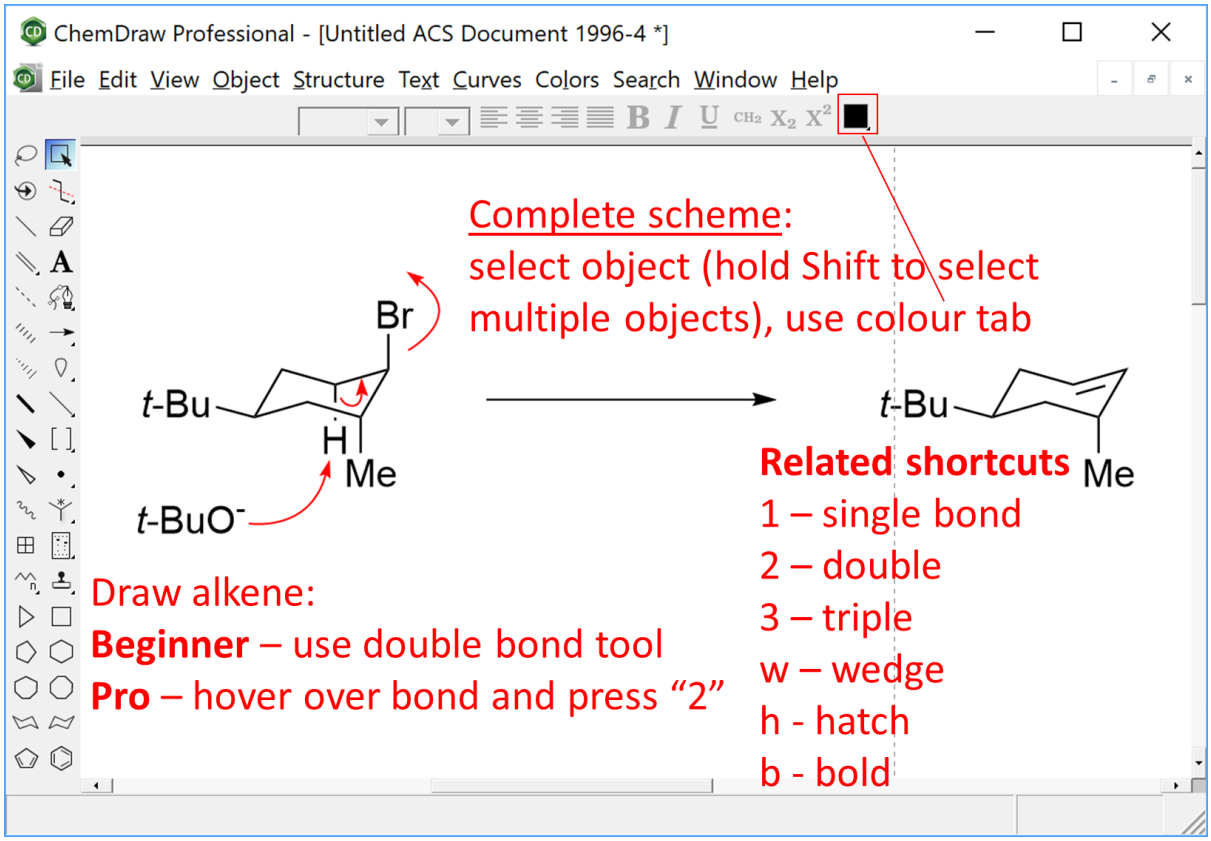
Drawing Your Curly-Arrow Mechanism

First need to draw your molecule in 3D chair-like conformation:




ChemDraw Professional - [Untitled ACS Document 1996-4 *]
File Edit View Object Structure Text Curves Colors Search Window Help
Br
t-Bu
H
Me
Br
t-Bu
H
Me
Bond should be at front:
select + F2 (F3 moves objects to back)


ChemDraw Professional - [Untitled ACS Document 1996-4 *]
File Edit View Object Structure Text Curves Colors Search Window Help
F7: zoom in
F8: zoom out
F9: superscript
F10: subscript
Br
t-Bu
H
Me
t-BuO⁻
Beginner: use arrow tools + pick curved arrows
Pro: use Edit Curve option – can make complex intricate curves, then select Curves>Full arrow at end



Well done - you're no longer a Chemdraw amateur!

Youtube has a large number of instructional videos if you want to learn more.

But if you want to be a master, need to use hotkeys:

Peter Knipe

November 2018

Appendix: List of Chemdraw Hotkeys

From Chemdraw version 16 user manual

Hotkeys are organized into atom labels, bond types, and functions (such as adding a charge or displaying a bond). Shortcuts are organized by the menu on which the command is found.

📝 ***Note:*** *You can modify hotkeys and nicknames. The tables in this section refer to the default values.*

Atom Keys

Use atom keys to insert atoms in a drawing using your keyboard. For example, place your mouse over an atom and press <**3**> to add a tert-butyl group.

Atom Label	Key
A	a
F	f
Ph	P or 4
Ac	A or 5
H	h
Q*	q
Br	b
I	i
R	r
n-Bu	1
K	k
S	s
s-Bu	2
Me	m
Si	S
t-Bu	3
N	n
TMS	t
Atom Label	Key
C	c
Na	N
X	x
Cl	C or l
O	o
COOCH3	E
D	d
OTs	T
CH2OH	6
Et	e
P	p
B	B

Bond Hotkeys

To modify a bond, place your mouse over the bond and select a key listed below.

Function	Key
Change to single bond	1
Change to dashed bond	d
Change to double bond	2
Change to wavy bond	y
Change to triple bond	3
Position a double bond to the left	l
Change to quadruple bond	4
Center a double bond	c
Change to bold bond	b

Function	Key
Position a double bond to the right	r
Change to wedged bond	w
Bring bond to front	f
Change to hashed bond	H
Open a bond properties text box	/ (slash) or ?
Change to hashed-wedged bond	h
Fuse 5 membered ring	5
Fuse 6 membered ring	6
Fuse 7 membered ring	7
Fuse 8 membered ring	8
Create chair form of cyclohexane with two different orientations	9 or 0

Function Hotkeys

To apply function hotkeys, place your mouse over an atom and press the appropriate key.

Function	Key
Add an attachment point	. (period)
Add an atom number	‘ (single quote)
Add a negative charge	-
Add a positive charge	+
Sprout one bond	0
Sprout two bonds	9
Sprout three bonds	8
Display the Atom Properties dialog box	/ (slash) or ?
Display the Choose Nickname dia-	= (equals)

Function	Key
log box	
Open an atom label text box	<Enter>
Remove an atom label	<Backspace>, <Delete> or <space>

Shortcuts

Below is a list of key combinations for common tasks.

File

Command	Key Combination
Create a new document	CTRL+N
Open a document	CTRL+O
Save a document	CTRL+S
Save a document as	SHIFT+CTRL+S
Print a document	CTRL+P
Page setup	SHIFT+CTRL+P
Close a document	CTRL+W
Exit ChemDraw	ALT+F4

Edit

Command	Key Combination
Cut	CTRL+X
Copy	CTRL+C
Copy as CDXML	CTRL+D
Paste	CTRL+V
Select all	CTRL+A
Undo	CTRL+Z

Command	Key Combination
Redo	SHIFT+CTRL+Z
Repeat last command	CTRL+Y
Clear	Clear
Copy as SMILES	ALT+CNTL+C
Copy as MOL text	ALT+SHIFT+CNTL+O
Paste as SMILES	ALT+CNTL+P
Paste as MOL/CDXML	ALT+SHIFT +CNTL+P

View

Command	Key Combination
Actual size	F5
Reduce	F8
Magnify	F7
Fit to window	F6
Toggle ruler	F11
Toggle crosshair	CTRL

Object

Command	Key Combination
Toggle fixed length	CTRL+L
Toggle fixed angles	CTRL+E
Select multiple objects	SHIFT+Click (with Lasso, Marquee, or Structure Perspective tools)
Group selected objects	CTRL+G
Ungroup objects	SHIFT+CTRL+G
Join selected objects	CTRL+J

Command	Key Combination
Bring to front	F2
Send to back	F3
Flip horizontal	SHIFT+CTRL+H
Flip vertical	SHIFT+CTRL+V
Rotate 180° horizontal	ALT+SHIFT+CTRL+H
Rotate 180° vertical	ALT+SHIFT+CTRL+V
Rotate... (opens Rotate Objects dialog)	CTRL+R
Scale...(opens Scale Objects dialog)	CTRL+K
Align left edges	ALT+SHIFT +CNTL+L
Align centers	ALT+SHIFT +CNTL+C
Align right edges	ALT+SHIFT +CNTL+R
Align top edges	ALT+SHIFT+CNTL+T
Align center towards top/bottom	ALT+SHIFT+CNTL+M
Align bottom edges	ALT+SHIFT+CNTL+B

Structure

Command	Key Combination
Clean up structure	SHIFT+CTRL+K
Convert name to structure	SHIFT+CTRL+N
Convert structure to name	ALT+CTRL+N

Text

Command	Key Combination
Flush left	SHIFT+CTRL+L

Command	Key Combination
Center	SHIFT+CTRL+C
Flush right	SHIFT+CTRL+R
Justified	SHIFT+CTRL+J
Automatic justification	SHIFT+CTRL+M
Plain	CTRL+T
Bold	CTRL+B
Italic	CTRL+I
Underline	CTRL+U
Formula	CTRL+F
Subscript selected character, or next character typed	F9 (in a label)
Superscript selected character, or next character typed	F10 (in a label)
Adds a degree sign (°)	ALT+248 (in a label)

Drawing

Command	Key Combination
Copy a selected object	CTRL+drag
Copy a selected object (constrained to X and Y axes)	SHIFT+CTRL+drag
Distort (limit resize to X or Y axis)	SHIFT+drag (with resize handle)
Toggle the Lasso and the previous drawing tool	CTRL+ALT+Tab
Change direction of a chain	CTRL+Drag (with alkane chain tool)
Change orientation of double bonds	SHIFT+Click (with saturated double-bond ring tools)
Create resonance delocalized ring	CTRL+Click (with ring tools except chairs)
Remove a curve segment	ALT+SHIFT+Click (with the pen tool)

Nicknames

Ac	Bz	c-C7H13	cyclopropyl	DPIPS	i-C4H9
Ad	BOM	c-C8H15	Cys	DPTBS	i-C5H11
Ala	Bs	c-Hx	Dan	DTBMS	i-Pr
Alloc	Bt	C10H20	DEAE	DTBS	Ile
Allyl	Btm	C10H21	DEIPS	Et	Im
Am	Bu	Cbz	DMIPS	Fmoc	Leu
Arg	Bzh	cHx	DMPM	Gln	Lys
Asn	Bzl	CoA	DMPS	Glu	m-C6H4
Asp	BzOM	Cy	DMTr	Gly	m-Phenylene
Benzoyl	c-C3H5	cyclobutyl	DNP	His	m-Tolyl
Benzyl	c-C4H7	cycloheptyl	Dnp	i-Am	MDIPS
Bn	c-C5H9	cyclooctyl	Dns	i-Bu	MDPS
Boc	c-C6H11	cyclopentyl	DNS	i-C3H7	Me

MEM	n-Pr	Phenyl	s-Butyl	TBDMS	Thr
Mes	N3	Pht	s-C4H9	TBDPS	TIPDS
Met	neo-Am	Piv	s-C5H11	TBMPS	TIPS
MMTr	neo-C5H11	PMB	SEM	TBS	TMS
MOM	Np	PMBM	Ser	TDS	Tos