nature portfolio

Style guide for chemical structures

Although there are a number of ways that chemical structures can be drawn based on individual preferences, our journals aim to use consistent styling wherever possible.

Presentation of chemical structures according to our style guidelines is not necessary for the initial stages of manuscript consideration, but we will work with authors to standardize the structures before final publication.

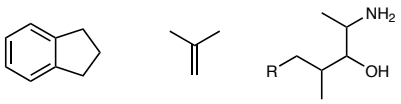
What follows is a list of preferences for structures that appear in *Nature*, the Nature Research journals (*Nature Chemistry, Nature Chemical Biology, Nature Nanotechnology,* etc.), *Nature Communications* and the Nature Reviews Journals (*Nature Reviews Chemistry, Nature Reviews Materials,* etc.)

Drawing chemical structures and structure-based figures using these preferences and the associated ChemDraw stylesheet will mean that less intervention by production editors will be required. This will result in fewer changes to the figure layout, consequently reducing the chances for errors to be introduced after acceptance.

We recognize that there are situations in which following these guidelines will not be possible. Some specific examples are given at the end of this guide; however, we recommend drawing all structures using the template as a starting point and modifying it accordingly if necessary or desirable. If, after reading this guide, you have any questions, please contact the specific journal for more information.

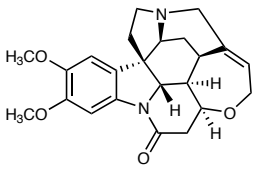
Bonds

- Standard bond angles should be used and made consistent throughout the manuscript when possible (exceptions can be made for 3D representations of molecules and complex polycyclic structures).

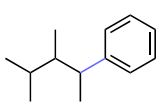


rather than:

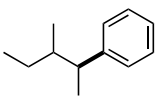
An exception:



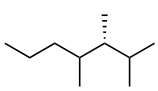
- Bond thicknesses should be consistent when possible. To emphasize a specific bond, consider using colour; bonds made boldface purely for emphasis can be mistaken for those indicating stereochemistry



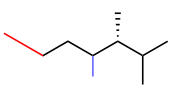
rather than:



- Bond lengths should be consistent throughout all figures when possible (although they may be manipulated to avoid having atom labels clashing with other labels or parts of the structure).

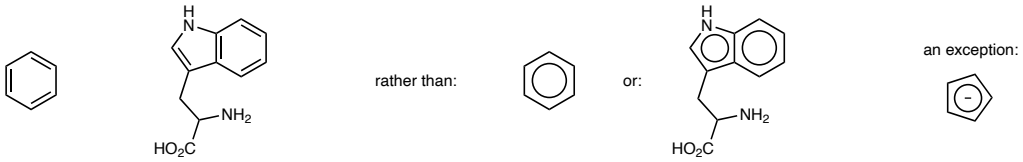


rather than:



The bonds shown in red and blue are too long and too short, respectively.

- Discrete bonds should be shown, rather than rings (some exceptions are OK, such as cyclopentadienyl anions).

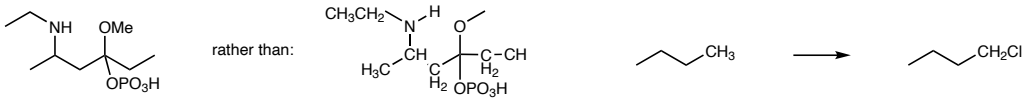


- Particular attention should be paid to structures generated by ChemDraw templates.

The bonds shown in red and blue are too long and too short, respectively.

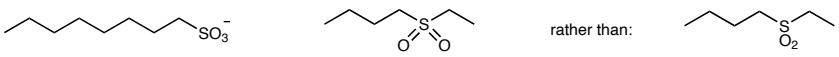
Atom Labels

- Only heteroatoms or groups that are altered during the course of a reaction should be labelled.

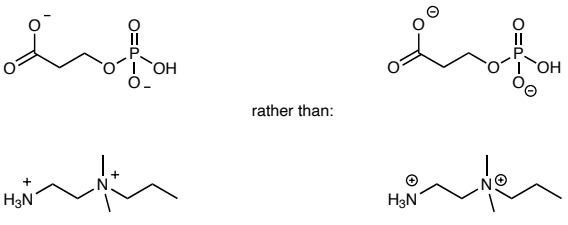


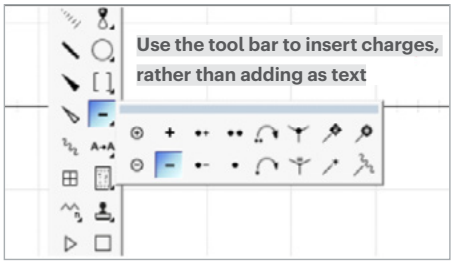
- Methyl groups should ideally be labelled as Me when attached to a heteroatom and denoted just as an unlabelled bond when attached to another carbon atom. Terminal methyl groups may be shown as CH_3 if necessary — but consistency is essential. Me, H or other labels attached directly to heteroatoms are not usually separated by a bond.

- Preferred abbreviations of common functional groups are: CO_2H, NO_3, NO_2, SO_2, N_2, N_3, OPO_3H (Pi and 'P' in a circle may also be acceptable abbreviations in certain reaction schemes), Ph, Ac, Bn, Me, Et, ^{i}Pr, Bu, ^{n}Bu, ^{t}Bu, Fmoc, Boc, Bz, Cbz, PG, LG, R, Nu, E (or E^{+}), X. Non-standard abbreviations should be defined. Abbreviations in the middle of a chain often introduce ambiguities (especially among non-experts), and so to maintain consistency throughout a series of figures, we recommend drawing out such structures.

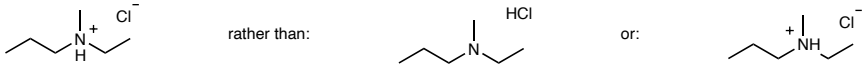


- Do not draw circles around charges. Plus or minus symbols for charge should reside on formally charged atom (i.e., $R_3N^{+}H$, not R_3NH^{+}), although their specific placement around the atom is flexible (see examples below). Use the charge tool rather than including the charge within the atom label. The size of the charge symbol is defined by font size, but often appears small. Consider enlarging charges for clarity.

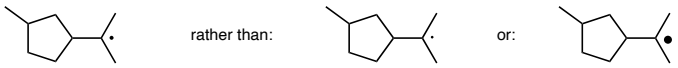




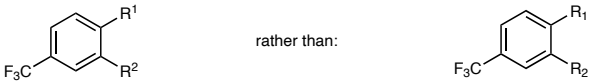
- Salts should be shown with counterions in dissociated form.



- Radicals should be visible, but not too large. As with charges, we recommend using the radical tool in ChemDraw and enlarging for clarity/visibility.

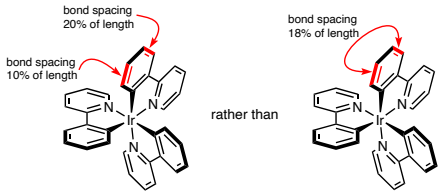


- When distinguishing R groups by including a number with the descriptor, the number should be a superscript, NOT a subscript. This avoids potential for confusion between different R groups and multiple R groups being appended to an atom.

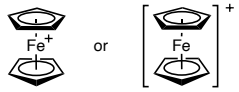


Organometallics

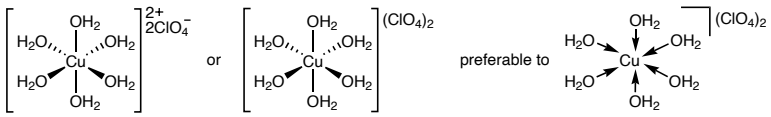
- Adjust the spacing between double bonds in aromatic ligands shown in perspective.
Change bond spacing to absolute value rather than percentage of bond length



- Charges on complexes can be shown at the metal atom or on the whole complex — but be consistent!



- Include counterions if possible, but be consistent in notation. Use dative bonds sparingly.



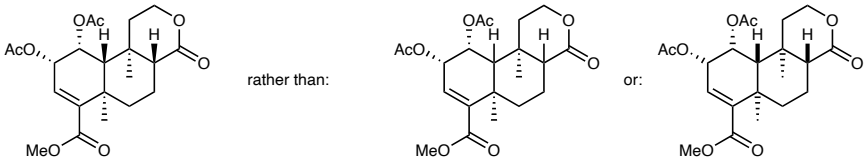
Stereochemistry

- Compounds that need extra definition include enantiomers, diastereoisomers and *cis* and *trans* isomers.

- **A cautionary note:** If you need to redraw a chiral molecule in a different orientation/arrangement or flip it in either dimension, be careful that the configuration of the original is the same as that of the original (flipping something in ChemDraw can often give you the mirror image of what you started with). We suggest using 'Show Stereochemistry' in the 'Object' menu to compare before and after structures.

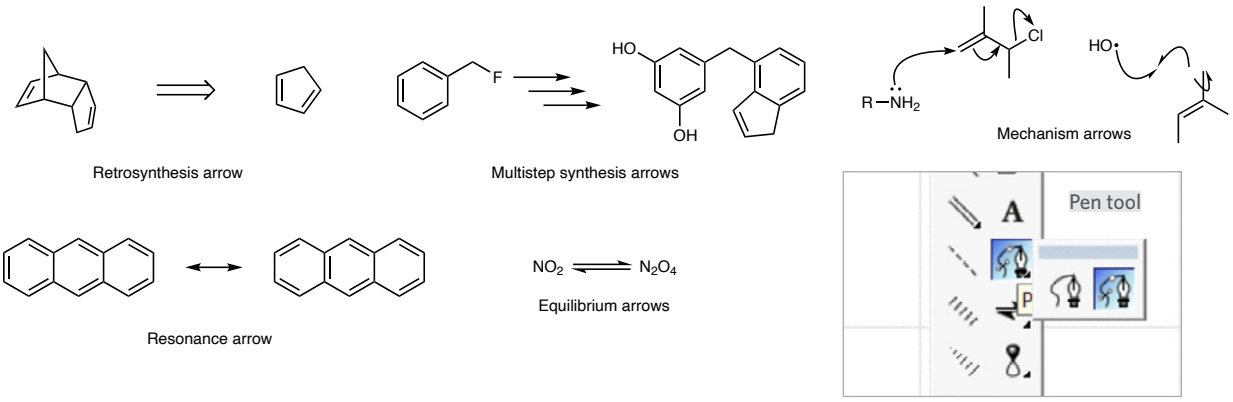
- Stereochemistry must be specified with boldface and dashed wedges. Omit hydrogens unless necessary to specify stereochemistry.

- Use wedges instead of thick bonds. The direction of wedged bonds does NOT indicate perspective; the narrow end of the wedge indicates the atom 'in the plane of the paper' for the purposes of absolute configuration determination at that stereocentre.



Arrows

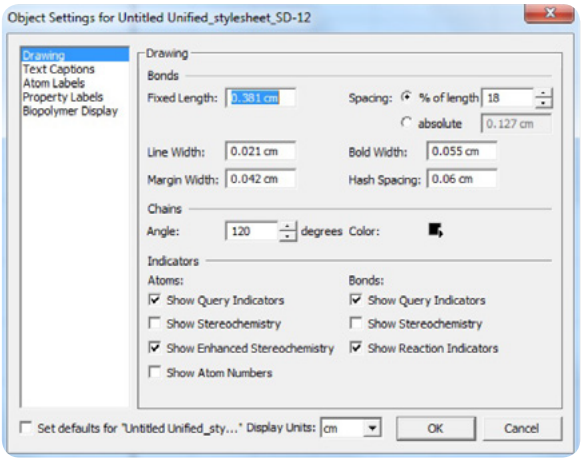
- Please use the types of arrows listed below for each indicated purpose.



- Curly arrows in mechanism diagrams should be shown going from the centre of a breaking bond or lone electron pair to the centre of a forming bond or a specific atom. We recommend using the pen tool to position arrows accurately rather than using the template curved arrows in ChemDraw.

Moving towards publication

- **Fonts/formatting** (these preferences are already set in the ChemDraw template):
  - Please use **Arial or Helvetica 6 pt** font for all atom labels.
  - Do not use boldface for atom labels. To emphasize a specific atom, consider using colour. Boldface should only be used for compound numbers and/or compound descriptors.
  - "Show Labels on Terminal Carbons" and "Hide Implicit Hydrogens" should be **UNCHECKED.**
  - Please use the following drawing settings:
    - **Fixed Length:** 0.381 cm
    - **Bond Spacing:** 18% of length*
    - **Line Width:** 0.021 cm
    - **Bold Width:** 0.055 cm;
    - **Margin Width:** 0.042 cm
    - **Hash Spacing:** 0.06 cm
    - **Chain Angle:** 120° bond spacing



**When drawing unsaturated rings in a tilted orientation, it may be necessary to re-adjust bond spacings to produce a structure that is pleasing to the eye.*

Formatting of text captions:

- Please use **Arial or Helvetica 6 or 6.5 pt** font.
- Use boldface and italics formatting sparingly. Boldface should only be used for compound numbers and/or compound descriptors. Use of italics should follow the accepted conventions.

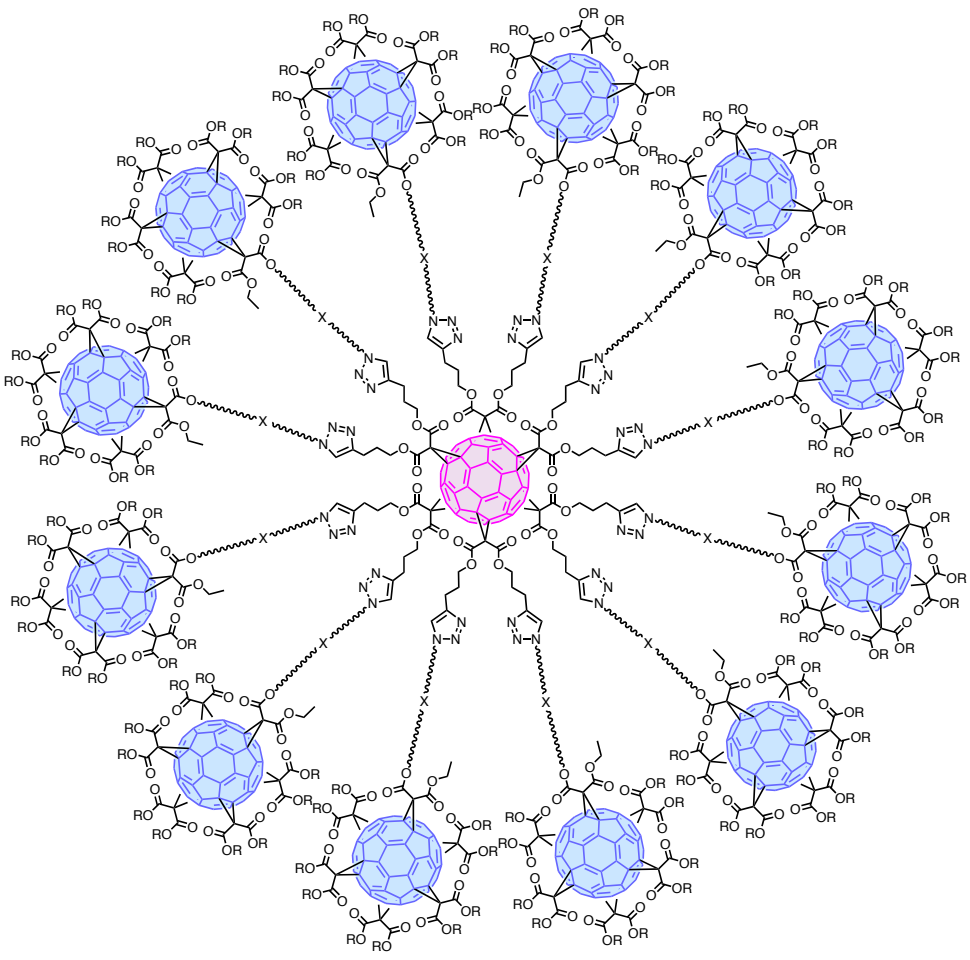
Warnings: ChemDraw provides the option of using several warnings to alert the user that there are too many or too few bonds to an atom, unbalanced parentheses, and similar. These are currently turned on in our template, and can be helpful in identifying places where there might be problems (although identifying the cause of the warning is up to you!). However, this warning system does not catch every problem, so please confirm the correct appearance of your structures according to the previous preferences and your chemical intuition.

Exceptions

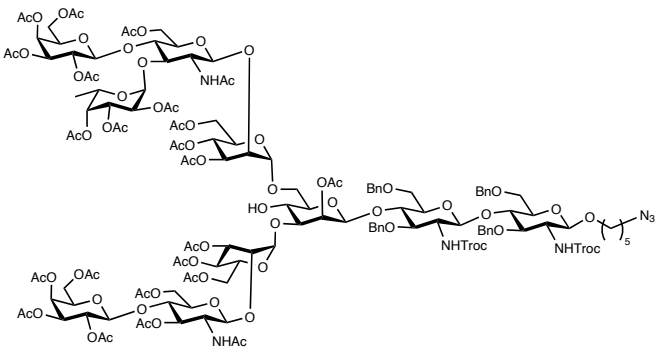
As with all good rules, there are some exceptions. The most obvious examples arise for large, complex molecules such as dendrimers that will not fit within the page limits if drawn using the standard settings.

In such cases we recommend that the structure is first drawn using the standard settings and then scaled down to fill the available width. Scaling should be performed within ChemDraw; bond widths and atom labels should NOT be scaled in the first instance.

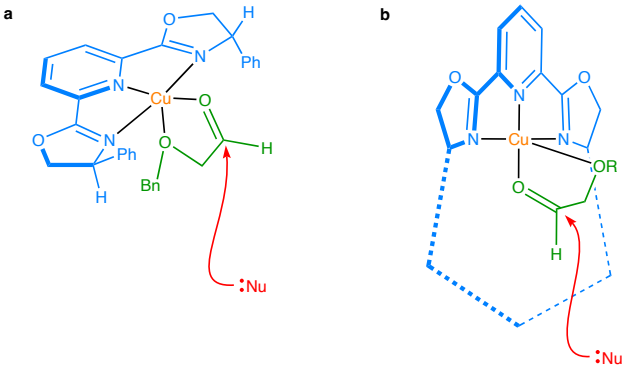
Atom labels may ultimately be scaled down to an absolute minimum of 5 pt.



Drawn using the standard settings, this large molecule would not fit within the page limits. The bond lengths were carefully adjusted, and the atom labels changed to 5 pt font. The line widths remain at 0.021 cm.



This molecule was just one part of a reaction scheme describing complex carbohydrate synthesis. The structure was scaled down to 83% of original size so that it would fit within the page constraints. Scaling down as in these two examples is not recommended on a regular basis because it comes at the expense of readability.



These structures were scaled up from the regular size because doing so afforded increased clarity in the mechanistic detail. The structures were first drawn at the regular size and then scaled up when it became apparent that space was available.