

## The ChemSketch windfall

*Cedric Mumford*

*ChemSketch* is a free computer program that can be downloaded from the Internet by teachers or pupils and used to construct chemical equations, molecular structures and laboratory diagrams with comparative ease. The program incorporates many advanced features such as the ability to view coloured, rotating molecules in space-filling mode. Ions, functional groups, complete molecules and apparatus can be selected from a large menu of templates and re-sized or moved to any point on a page. The package includes text and drawing tools. Here the author shows how to construct some sample molecules and mathematical equations using *ChemSketch*.

Computer programs for use in chemistry can be expensive, time-consuming to learn, exasperating to use, and sometimes lacking in the combined text, mathematical and drawing tools needed to produce quality hand-outs. Even the type of computer available can limit access to good programs.

For a project at the University of Wales Institute,

Cardiff (UWIC) I needed a program I could learn to use quickly and to a high standard. While looking at the chemistry programs posted on the net, *ChemSketch 5.0* dropped like a windfall from hyperspace. The program, available as a free download from the Canadian company ACD Labs (see 'Website'), met my requirements. It is intuitive in use, has many ready-to-use templates and includes excellent word-processing and drawing packages. Undoubtedly its most eye-catching feature is its ability to show molecules as coloured objects rotating in space. This feature will sway students who think chemistry is abstract, and even those whose inclination is towards art will be stimulated. Imagine molecules made into cushions!

### Downloading and modes

*ChemSketch* takes about an hour to download on a home computer. The program opens with *Tip of the day*. The tips point to tools available through the

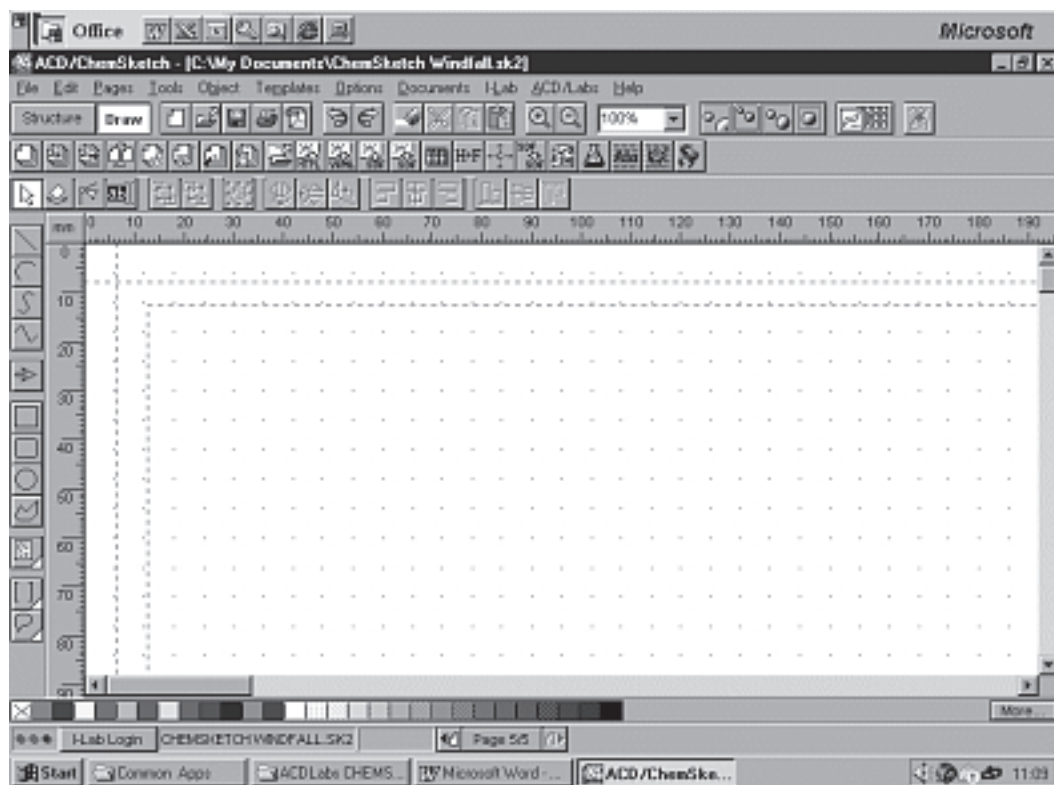


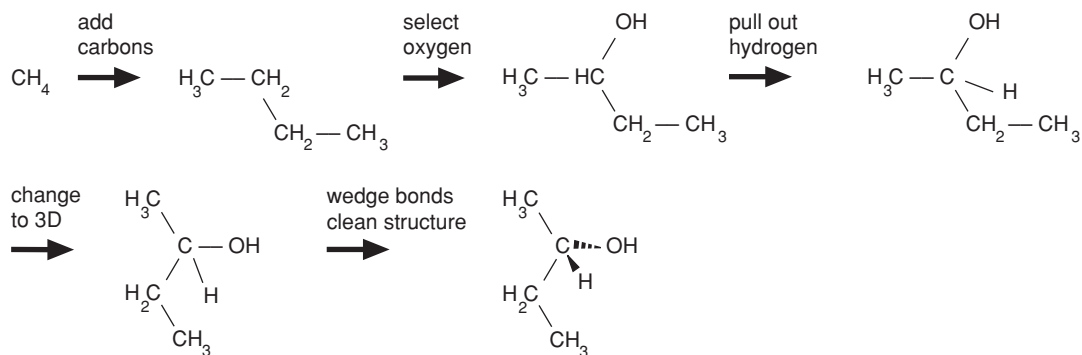
Figure 1 The *ChemSketch* toolkit.

excellent *Help* list, but deliver these in manageable portions. It is important to notice that the program operates in two modes, *Structure* and *Draw* (Figure 1). *Templates*, including amino acids, aromatics, ring structures, carbohydrates and anions, are available in both modes. The *Lab kit* template contains seven pages of common laboratory apparatus, including a distillation set-up, volumetric equipment and sets of Quickfit glassware, that can be selected, moved and fitted together as needed. One of two selection tools allows the user to shrink equipment to fit the space available; the other tool allows thermometers and dropping funnels to be rotated to fit flasks with angled necks.

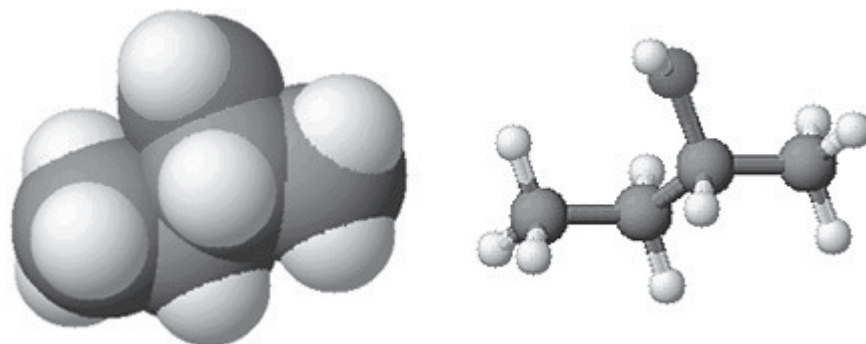
## Constructing molecules

In *Structure* mode the user can construct molecules. Double and triple bonds are made to appear by repeatedly clicking on the relevant bond. Stereo-bonds can also be inserted. Roughly drawn molecules can be tidied using the *Clean structure* tool. Other tools allow the structure to be rotated in the plane of the screen. Selecting the menu title *ACD/Labs* and then *3-D Viewer*, allows the drawn molecule to be viewed in several styles, for example as a coloured space-filling model.

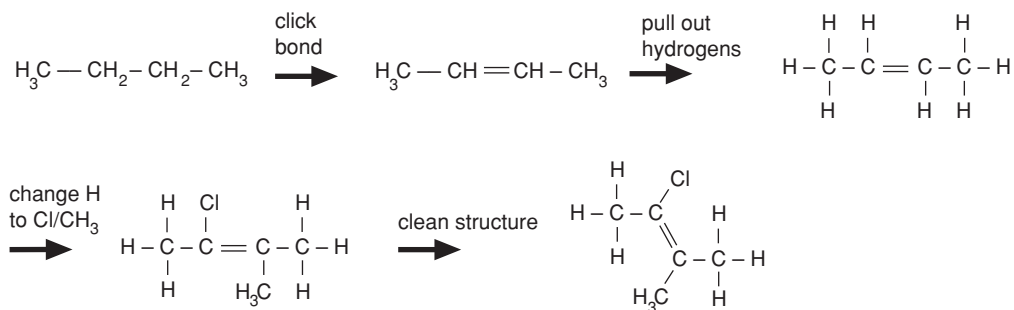
Scheme 1 shows the stepwise construction of butan-2-ol. Figure 2 shows this molecule in the 3-D viewer as both a space-filled and a stick model. If desired, C–H bonds can be drawn at 90° angles by selecting H from the atoms menu, selecting the relevant carbon and dragging H to the desired place (Scheme 2). Halogens and other atoms are inserted by selecting the required atom from the *Atoms* menu and then clicking on the hydrogen atom to be replaced. The *Template* tool includes a file of carbon radicals and small rings that can be added to molecules under construction (Scheme 3).



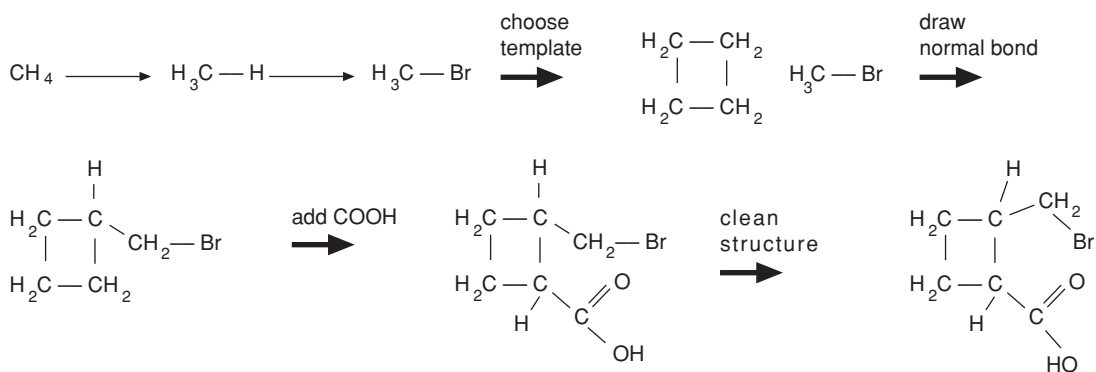
**Scheme 1** Construction of butan-2-ol.



**Figure 2** 3-D views of butan-2-ol.



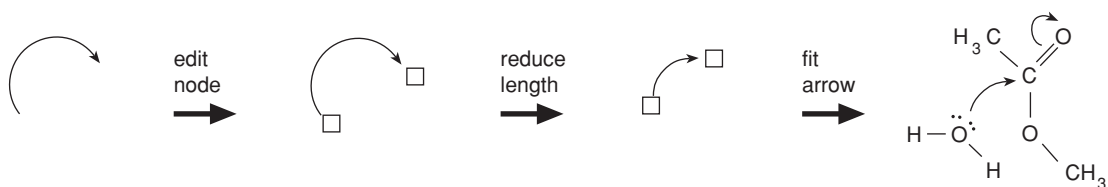
**Scheme 2** Construction of 2-chloro-3-methyl but-2-ene.



**Scheme 3** Constructing 2-bromomethylcyclobutanoic acid.

## Drawing tools

In *Draw* mode there are tools for straight and curved lines, circles, squares and a variety of arrows and half-arrows needed in chemical equations. By clicking on tools for both curved lines and arrows it is possible to draw curly arrows and half arrows. Producing curly arrows of the correct length, curvature and position takes practice and some patience. A useful tool for this purpose is *Edit nodes*. Begin by drawing an arrow of the desired curvature in an empty space and use *Edit nodes* to adjust its length. Then move the arrow to its intended place in a chemical structure. Finally, if necessary, use the *Select/Move/Rotate* tool to adjust the angle (Scheme 4).



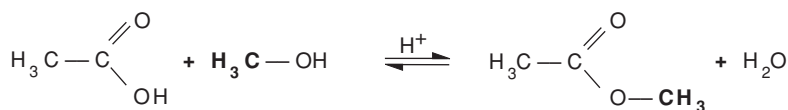
In this scheme the lone pairs of electrons on oxygen were selected from the *Reaction Symbols* template. Other symbols include:



**Scheme 4** Attack of water on an ester.

Three extremely helpful tools are the ones for superscripts [<sup>s+</sup>] subscripts [<sub>s</sub>] and *Object/Group*. The subscript and superscript tools are turned on by clicking on the toolbox in advance of typing a symbol or numeral and turned off again by re-clicking the same tool. The *Group* tool is used in *Draw* mode and locks together a number of highlighted structures and symbols as *Objects*. The group can then be re-sized or moved as one unit for positioning on a page or exporting to *Word* documents. If necessary, the group can be *Ungrouped* for editing purposes.

Inevitably the user makes mistakes in using *ChemSketch*, the most common being to deposit CH<sub>4</sub> in an unwanted place or to delete the wrong structure using the *Delete* tool. The *Undo* tool in the form of a curved backward arrow will undo up to 50 consecutive errors. Moreover, structures can be selected for editing or deleting by a click near the structure so that an enclosing box appears. Deselection is done by clicking outside the selection box. Particular atoms and groups in a structure can be highlighted and deleted by pointing with the *Delete* arrow. The same highlighted features can be emboldened, or the colour changed, using the *Properties* dialogue box in *Tools/Structure/Properties*. Text colours can be changed using the *Tools/Pen Style* panel. This emphasis is useful in showing where groups end up in reactions (Scheme 5).



**Scheme 5** Highlighting groups in a reaction.

Ionic equations are easily written, and there is a template of inorganic and organic anions. If the superscripted negative sign proves too small a short line can be drawn instead and repeated by copying and pasting as required (Scheme 6).

In *Structure* mode



In *Draw* mode



**Scheme 6** Writing ionic structures and equations.

Copying and pasting is useful where structures, diagram or symbols need to be repeated exactly. *Paste-in-place* works for drawn objects, and *Paste structure* is best for chemical structures. A shadow of the copied structure is seen that is very helpful in positioning items within a page.

## Mathematical equations

*ChemSketch* lacks a full set of mathematical symbols, but integration signs and the line separating numerators from denominators can be drawn using the *Line* and *Curve* tools (Scheme 7). Greek letters can be written by going into *Tools/Font panel/Symbol* and typing an Arabic equivalent (e.g. *q* for  $\theta$ ). Numerators and denominators should be typed in a narrow text box and then moved into place. Square-root signs can also be drawn and moved into place.

$$\begin{array}{ccc}
 \frac{1}{2} & \xrightarrow{\text{combine}} & \frac{1}{2} & \xrightarrow{\text{repeat using smaller font}} & \frac{1}{2} \\
 \int & \longrightarrow & \int_0^{\cos^{-1}(2E/\mu V)^{\frac{1}{2}}} & \sin\theta \cos\theta \delta\theta = & \frac{1}{2} \left(1 - \frac{2E}{\mu V^2}\right)
 \end{array}$$

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**Scheme 7** Mathematical equations.
 

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*ChemSketch* contains many advanced features beside those described here. Using the program is a process of discovery that constantly delights and surprises the user. With downloads now in excess of 100 000 copies, it has proved its popularity across the globe. *ChemSketch* is being used in transferring a set of chemistry notes to the UWIC server. These notes fill specific gaps in students' knowledge and were previously photocopied from originals in which chemical structures and diagrams were hand-drawn. Using *ChemSketch* to produce these notes means that any future editing will be easy.

**Acknowledgement**

The author thanks David Campy for his helpful suggestions and efforts in producing this article and in transferring the files of chemistry notes to the UWIC server.

**Website**

ACD Labs: <http://www.acdlabs.com/download/chemsk.html>

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**Cedric Mumford** FRSC retired in January 2002 from 30 years of teaching applied chemistry in the School of Applied Sciences, University of Wales Institute, Cardiff. E-mail: [cmumford@uwic.ac.uk](mailto:cmumford@uwic.ac.uk)

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