Chemistry by Interactive 3D

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Chemistry has high conceptual content, in that
observations require interpretation, while:
interpretation is generally in terms of
intangibles, such as atoms and molecules;
many concepts are presented in mathematical
terms which require interpretation;
and
graphical presentation is often integral

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Pictorial Graphics

Graphical images may be simple pictures of 2D and 3D objects, e. g., apparatus

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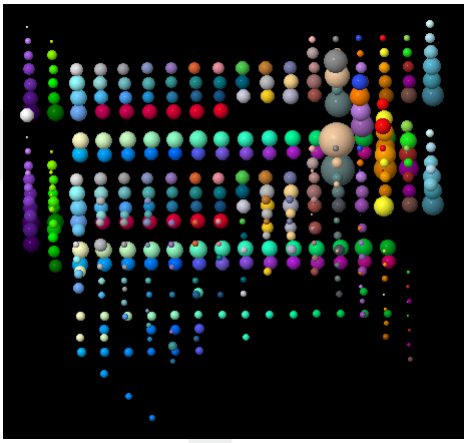
Pictorial Graphics

Graphical images may be in static form, e. g., a graphical Periodic Table by Angel Herráez.



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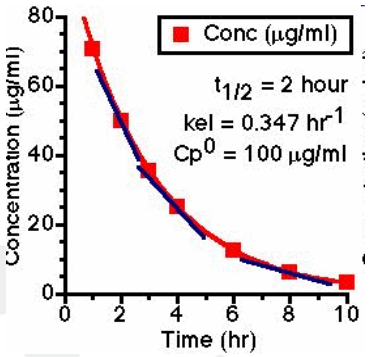
Graphs

Graphical images may be two-dimensional graphs, e. g., concentration *versus* time.



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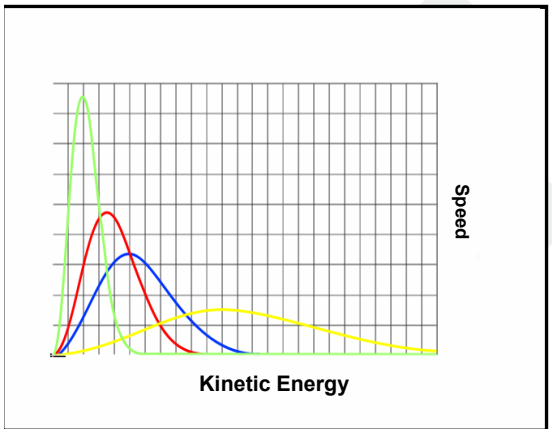
Graphs

But two-dimensional graphs may actually be projections of 3D data



for example: speed *versus* energy for different noble gases.

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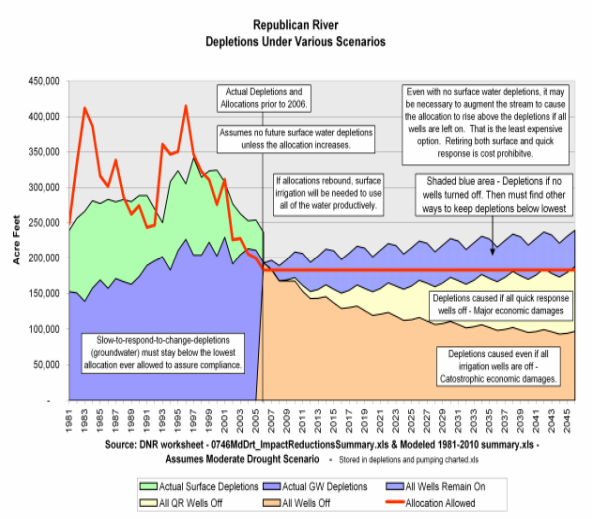
Graphical Complexity



And increasing complexity adds to the difficulties in comprehending graphics

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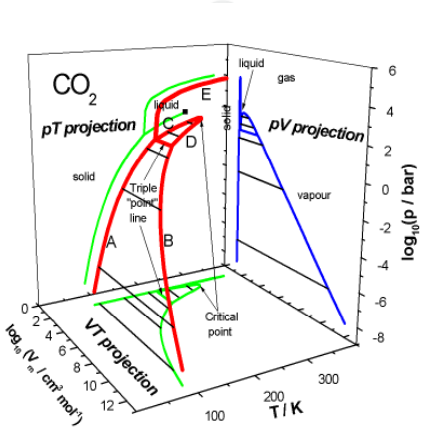
3D Presentation



Difficulties are addressed on paper or screen by adding features to the graphic, such as attempts at 3D presentation (orthographic or perspective) and colouring.

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Modern computer graphics has expanded the possible modes of presentation many-fold, permitting images to be manipulated in various ways, such as interactive involvement and animation.

We will explore some of the current and developing methods of image manipulation, firstly for molecular systems and then for graphical presentation.

Modes of Presentation

There are many specialist stand-alone programs for graphics

but

there is an increasing focus on web-based programs which require neither purchase nor installation.

An important such program is the Java-based Jmol.

Jmol is available both as a stand-alone program and as a server-based application, where a Web browser can pick up both the program and its associated data remotely, in order to provide a local display.

Initially, Jmol* was used to produce interactive and animated molecular displays.

* = Web source

These displays can be of rapidly increasing complexity:

protein backbone*

protein strands*

animation*

protein cartoons*

some capabilities of Jmol

Crystal Structures may also be displayed:

C (graphite) and C (diamond)

#NaCl (halite)

#FeS_2 (pyrite)

#These diagrams are from the Virtual Museum of Minerals and Molecules.

However, there is much more to chemistry than structure!

We have recently developed a general Jmol graphics capability by which it has become possible to display general 3D objects.

plot functions*

phase diagrams*

Jmol is not the only system capable of displaying functions online.

Mathematica

Abstract

Chemistry is a visual, even tactile, science but is based upon fundamental concepts, such as complex molecular and crystal structures as well as mathematical descriptors, which are often difficult to appreciate. Interactive three-dimensional (3D) visualisation provides a tool by which such concepts are more readily grasped, by user manipulation of images in various ways (such as rotation, expansion to focus in certain areas, projection onto one of the three planes, measurement, colouring, labelling, etc.).

Jmol is Java-based open-source software, run by most Web browsers, initially for displaying molecular structures. However, in recent years, Jmol has been greatly expanded to manage data in 3-coordinate space, among other features. We demonstrate the use of Jmol (and others) in display and manipulation of images of various kinds: molecular and crystal structures, phase diagrams, mathematical functions, etc. These features and images are readily and freely available to add interest, immediacy and depth of understanding to teaching (and not only of chemistry) at all levels.