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Jmol – a paradigm shift in crystallographic visualization

Robert M. Hanson

Department of Chemistry, St Olaf College, 1520 St Olaf Avenue, Northfield, Minnesota 55057, USA. Correspondence e-mail: hansonr@stolaf.edu

Recent advances in molecular and crystallographic visualization methods are allowing instructors unprecedented opportunities to enhance student learning using virtual models within a familiar web-browser context. In step with these advances, the latest versions of the *Jmol* molecular visualization applet offer capabilities that hold potential for revolutionizing the way students learn about symmetry, uncertainty and the overall enterprise of molecular structure determination.

1. Introduction – crystallographic visualization

It goes without saying that visualization is important in the area of crystallography. The introduction of *ORTEP* (Johnson, 1965) over 40 years ago made possible for the first time a ready two-dimensional projection of the three-dimensional atomic world of crystals and ushered in a revolution in molecular visualization. Since then, personal computing power has increased immensely, and a number of computer programs have been introduced that allow real-time interactive construction of crystals (*CrystalMaker*, 2009; *Shape*, 2009) and exploration of molecular structure and bonding in the context of databases [*Mercury* (Macrae *et al.*, 2006) and *Diamond* (2010)]. While developed primarily for research purposes, these programs have found utility in the area of education as well, as noted in recent symposia at national American Chemical Society meetings (Kantardjieff, 2005; Battle *et al.*, 2009). In addition, specialized software and web-based tutorials specifically targeting fundamental concepts of crystallography and molecular symmetry are now available (Cass & Rzepa, 2005; Harwood & Korkmaz, 2005; Johnston, 2005, 2008; Charistos *et al.*, 2005; Kastner *et al.*, 2000).

This paper focuses on a new paradigm of computer program that aims to revolutionize the area of visualization in chemical education again, particularly in the area of crystallography. These programs – web-based, open-source and platform-independent – combine features of rapid development, expert communities and widely accessible databases with the power of the web to communicate features of molecular and crystallographic structure in creative and artistic ways that could not have been imagined in 1965. The paradigm shift of the 21st century is away from monolithic programs that are designed to do a specific task on a specific platform in a specific subdiscipline of science and toward tools that are more modular, flexible and useful in a broad interdisciplinary context. The shift is away from licensed profit-driven software with periodic updates to openly available software with rapid community-based 'immediate' development goals.

The *Jmol* molecular visualization applet (*Jmol*, 2010) is leading the way in this shift. We have just recently begun to learn how it can be used to enhance student understanding of the principles of crystallography and appreciation of the beauty of symmetry. The *Jmol* applet represents the third stage of an evolutionary process that started with the development of *RasMol* (Sayle & Milner-White, 1995) in 1989. This program, probably more than any other, brought the world of crystal structure into the hands of educators. Focused as it was on biomolecular structures, *RasMol* represented a major advance in the area of biochemistry and molecular biology. One of the important features introduced in *RasMol* was the capability of scripting, thus allowing for a 'guided tour' approach to exploration of crystal structures and opening entirely new possibilities for education.

With the development of the web during the 1990s came the second phase of this process, spearheaded by the release of the *Chime* Netscape plug-in in 1996. The *Chime* plug-in was essentially *RasMol* for the web with a broader focus that included calculated structures of small molecules. Educators with a bit of web-development experience could for the first time make available to a wider audience interactive molecular structure-annotated texts. Despite its limitations, *Chime* formed the basis of many tutorials and web-based educational software tools.

2. The *Jmol* molecular visualization project

The *Jmol* molecular visualization project, one of the early open-source projects of the 1990s, really came of age in 2002 when it became the *de facto* replacement for *Chime*, which had lost its commercial development support, was not released to the public domain and could not keep pace with the rapidly developing browser market. In contrast to *Chime*, *Jmol* presented the opportunity for a rapidly developing program within a dedicated community of users and developers,

Jmol has in the past several years grown from its initial focus as a web-based *RasMol*/*Chime* replacement into a

powerful visualization and analysis tool that remains highly modular and customizable. Unlike the other programs of the previous century, *Jmol* is essentially a massive easily accessible toolbox that can be used at the lowest level by dedicated professional Java programmers wanting to integrate molecular visualization into larger projects, at a more common level by scientists and educators wishing to communicate information *via* the web, and, finally, by students with little or no web design experience in the context of class projects, tutorials and laboratory exercises.

In terms of crystallography and education, now as we start into the second decade of the 21st century, *Jmol* offers its community of developer/users a wealth of ever-expanding capabilities. Some of these capabilities are highlighted below, most deriving from suggestions made by the *Jmol* user community within just the past few years. Mostly it is hoped that this paper will spark interest in finding additional ways *Jmol* can be of service to the wider crystallographic community both in education and in research. Capabilities discussed include file reading, script-based atom selection and display, analytical capabilities including measurement and surface analysis, and output options.

It is important to understand that there are three ways that *Jmol* can be utilized. These include a stand-alone Java program, a library of Java 'classes' and an applet for the web. Thus, *Jmol* can be used as a stand-alone program, much like the aforementioned programs. It can be used as a programming library that can be integrated with another program to provide molecular visualization. However, the real niche for *Jmol* is that it can be used as an applet in a web-based setting.

All of the features discussed below relate to all of these uses. However it is the integration of *Jmol* into a web page that offers the most for education, as that context provides an easy means of packaging a crystal structure into a broader educational objective.

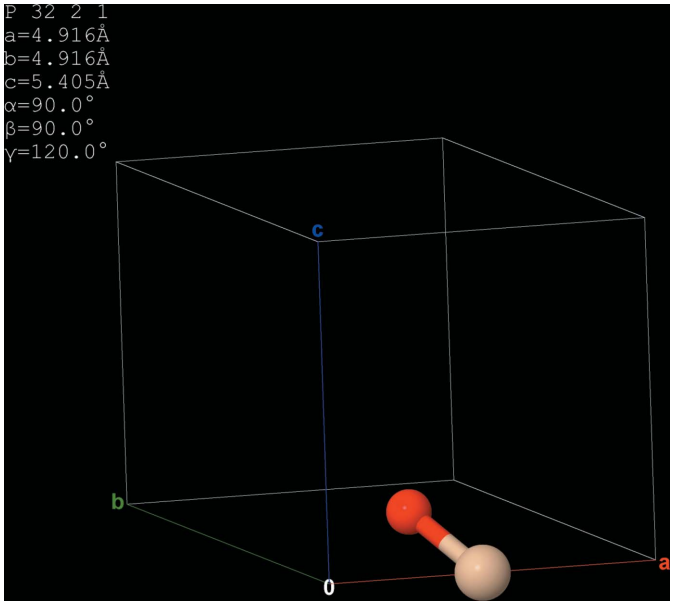

Figure 1
Quartz file data loaded without symmetry (`load quartz.cif`). The default loading does not apply symmetry, only creating atoms in the positions specified in the CIF.

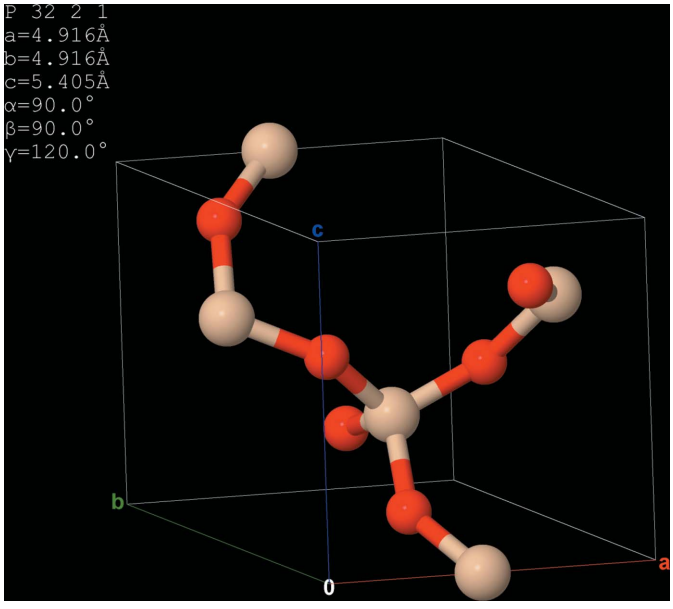

Figure 2
Quartz file data (Levien *et al.*, 1980; http://rruff.geo.arizona.edu/AMS/xtal_data/CIFfiles/00788.cif) loaded with symmetry applied, but not packed (`load quartz.cif {1 1 1}`). Symmetry operations that would create atoms in an adjacent unit cell are 'normalized' to move those atoms back into cell 555.

3. File-reading capabilities of *Jmol*

Probably more than any other broadly featured program in common use, *Jmol* includes an ever-expanding set of 'readers' that can open just about any structure file of interest. In particular, *Jmol* can read standard *SHELX* (Sheldrick, 2008), PDB (Protein Data Bank; Berman *et al.*, 2000), CIF and mmCIF formats, including crystallographic unit-cell, symmetry operator and anisotropic displacement parameters. Additional file formats of interest within the crystallographic community that are supported include files generated by the programs *FHI-aims* (Blum *et al.*, 2009; http://www.fhi-berlin.mpg.de/aims), *CASTEP* (Segall *et al.*, 2002; http://www.castep.org), *CRYSTAL* (Dovesi *et al.*, 1989), *VASP* (Jurgen, 2008; http://cms.mpi.univie.ac.at/vasp) and *WIEN* (Blaha, 1990; http://www.wien2k.at). *Jmol* recognizes space-group symmetry in terms of Jones–Faithful (x, $-y$, $z + \frac{1}{2}$) format, Hermann–Mauguin space-group names, Hall (1981) symbols and *International Tables for Crystallography* space-group numbers. Symmetry can be applied or not, and virtually any number of unit cells can be loaded at will using a simple script syntax (Figs. 1–7; interactive versions of all figures, and the data files used to generate these figures, are available as supplementary material[1]).

[1] Supplementary material for this paper is available from the IUCr electronic archives (Reference: KK5066). Services for accessing this material are described at the back of the journal.

Fig. 6 illustrates one of the unique features of *Jmol*: that one can load a crystal structure file and override the file-based crystallographic parameters associated with it. One can, for example, load a CIF into *Jmol* and then only apply a single Jones–Faithful operator – or, for that matter, apply any operator of any kind just to see what it does. One can quickly experiment with different members of a space-group family to see incrementally how the symmetry operations combine to form the overall symmetry of the system.

A further application of this feature is seen in Fig. 8. In this case, a standard *XYZ*-format file with just the minimum of structural information was 'loaded' into a unit cell, and arbitrary symmetry was applied. This feature of *Jmol* holds great

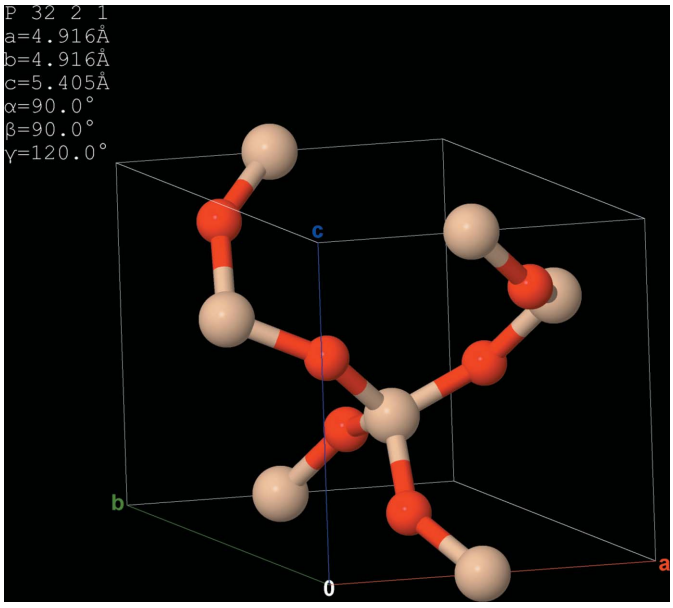

Figure 3
Quartz file data loaded as a packed unit cell (`load quartz.cif PACKED`). All atoms that are within unit cell 555 or an associated vertex, edge or face are included.

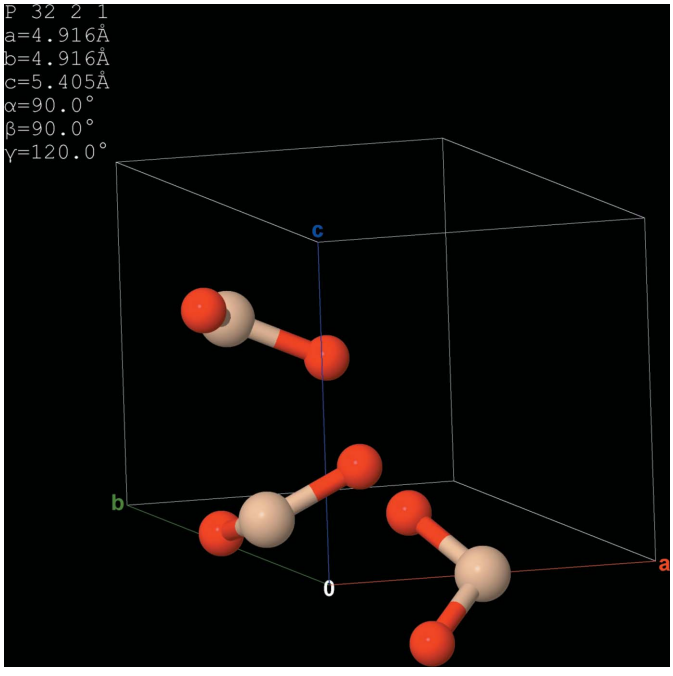

Figure 4
Quartz file data loaded with exact application of symmetry operators (`load quartz.cif {555 555 0}`). Only four of the nine atoms are contained within cell 555. In this case, there are six symmetry operators, including the identity operation. Note that the Si atoms (large) are in special positions and are generated by two symmetry operators each, while the O atoms (small) are in general positions.

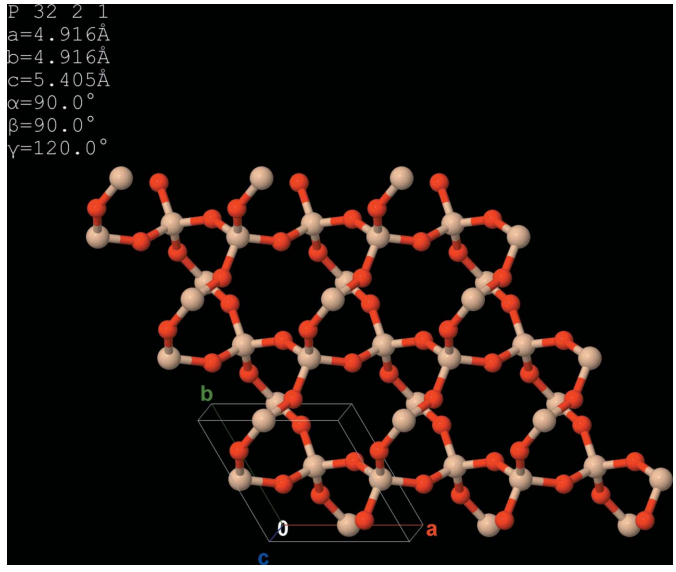

Figure 5
Quartz file data loaded as a set of nine unit cells (`load quartz.cif {3 3 1}`). With a little effort, the left-handed spiral chirality of the quartz crystal can be seen in the direction of the *b* axis.

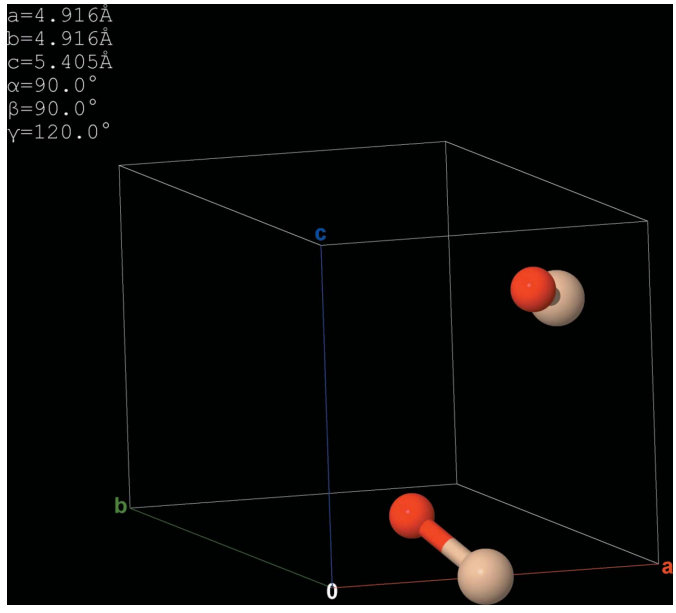

Figure 6
Quartz file data loaded with just one of its threefold screw axis operations (`load quartz.cif {1 1 1} SPACEGROUP "-y,x-y,z-1/3"`). This mode can be used to investigate the operation of any subset of symmetry operations within a space group.

potential to form the basis of a tutorial in symmetry using simple molecules or molecular fragments, allowing a student to experiment with different space groups, unit-cell dimensions and symmetry operators in real time.

4. General *Jmol* capabilities relating to crystallography education

Jmol's scripting capability makes it perfectly suited to an educational environment. Any educator with a bit of interest, and, probably, with help from the *Jmol* user community, can easily construct web pages that focus on specific topics relating to crystal structure. Through the use of trivially implemented associated standard web 'widgets' (buttons, links, selection boxes, text entry boxes *etc.*) a web page can be constructed in very short order that can allow quite a powerful educational experience. With some additional web savvy, an educator can produce a very professional piece of interactive technology focused on student learning.

What follows is a quick look at some of the features of *Jmol* applet scripting that are particularly suited to crystallography. This is by no means an exhaustive look at *Jmol* scripting. The interested reader is referred to the *Jmol* interactive documentation website (http://chemapps.stolaf.edu/jmol/docs) for a full list of *Jmol* scripting capabilities.

4.1. Atom selection

Jmol has extensive capability to select, display, highlight, move and hide particular sets of atoms. Specifically in relation to crystal structure, when a structure is loaded, *Jmol* retains information about the symmetry origins of the atoms. So, for example, one can select only those atoms that arose by a specific symmetry operation using `select SYMOP=3`. One can query *Jmol* as to what that symmetry operation is using `show SYMOP 3`, and one can explore the entire set of symmetry operations of a molecule using `show symmetry` or `show spacegroup`. Atoms within a specific unit cell can be selected using, for example, `select cell=555`.

4.2. Fractional coordinates and crystallographic atomic properties

Jmol scripts can refer to standard Cartesian coordinates as {*x y z*} or to fractional coordinates using at least one slash character as part of that description: `draw arrow {1/2 1/2 1/2} {1 1 1/1}`. In addition, *Jmol* can be queried for atom properties, among which include fractional coordinates *fx*, *fy*, *fz* and *fxyz*, and normalized unit-cell coordinates *ux*, *uy*, *uz* and *uxyz*. The print command along with formatting is a powerful mechanism of querying *Jmol* for all sorts of information. For example, `print {cell=555}.uxyz` reports the average unit-cell position for the atoms in the primary unit cell, and the command `print {*}.label("%a%i\t%5.3fx \t%5.3fy\t%5.3fz")` delivers a formatted list of atom names and numbers along with their fractional coordinates (Table 1).

4.3. Additional properties

Additional crystallographic properties of atoms that can be queried are given in Table 2. Most of these properties can be tabulated, compared, and applied as colors to molecular

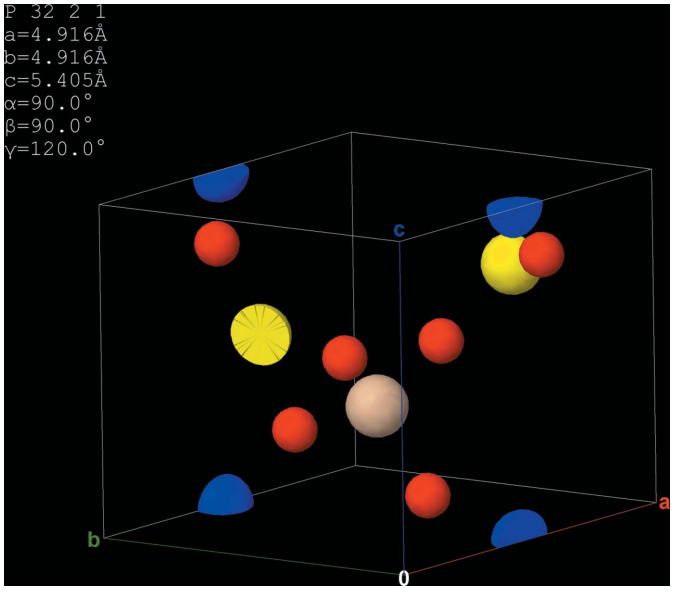

Figure 7
Packed and capped quartz unit cell where atoms having different fractions within the unit cell are shown with a different color and shape (small red: oxygen; other colors: silicon), demonstrating the unit-cell formula Si_3O_6 and empirical formula SiO_2 (`load quartz.cif packed; wireframe off; color {_Si} blue; color {atomno=6} none; color {atomno=3 or atomno=13} yellow; lcaoCartoon cap unitcell cpk; spacefill off`).

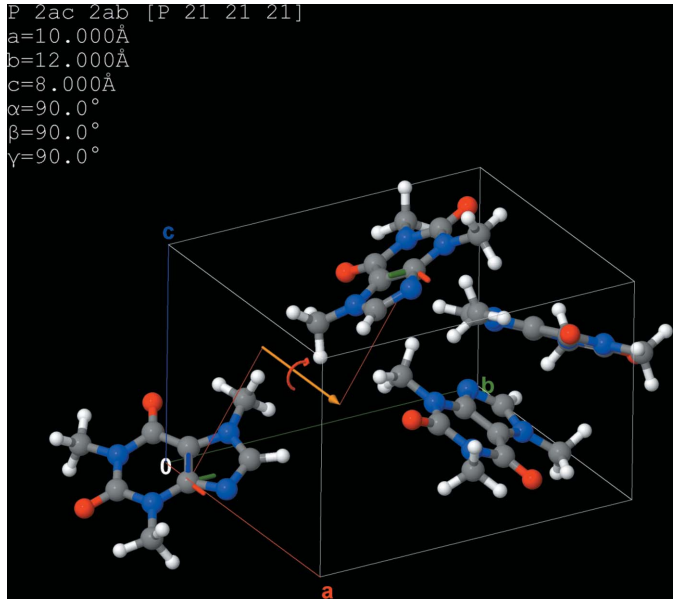

Figure 8
Caffeine model loaded as though it were packed in a crystal having orthorhombic space group $P2_12_12_1$. The twofold screw axis parallel to the *a* axis is shown (`load caffeine.xyz {1 1 1} spacegroup "P 21 21 21" unitcell {10.0 12.0 8.0 90 90 90}; draw symop {atomno=7} {atomno=55}`).

Table 1
A formatted listing of fractional coordinates for quartz.

Si1	0.470	0.000	0.000
O2	0.414	0.267	0.119
Si3	0.000	0.470	0.667
O4	0.267	0.414	0.548
Si5	1.000	0.470	0.667
O6	0.733	0.147	0.786
Si7	0.530	0.530	0.333
O8	0.587	0.853	0.214
O9	0.853	0.587	0.452
Si10	0.470	1.000	1.000
O11	0.147	0.733	0.881

surfaces or as sizes of atoms in order to highlight anomalies. The configuration property is interesting in that it allows the user to display specific disorder sets (`display configuration=1`) or a superposition of configurations (`display configuration=0`) (Figs. 9 and 10).

4.4. Visualization of symmetry

One of the more recent and exciting areas of development of *Jmol* has been in the area of visualization of symmetry elements. Planes and axes are easy to produce in *Jmol* using, for example, `isosurface plane x=3; draw axis {0 0 0} {0 0 1/1}`. Given a specific unit cell, one can draw the intersection of planes in a natural fashion (Fig. 11).

Most interesting by far, though, is the ability of *Jmol* to depict complex relationships between two atoms or between two molecules such as glide planes and screw axes in a relatively simple fashion. These elements of symmetry are by far the most difficult to visualize, but with *Jmol* they are trivial to produce based on symmetry operators present in the file or added by the user. So, for example, if symmetry operator 2 is $(-x, y+\frac{1}{2}, -z+\frac{1}{2})$ (a twofold screw axis with translation along the *b* axis), then `draw symop 2 {1/4 0 1/4}` will depict that operation applied to an atom at position $(\frac{1}{4}, 0, \frac{1}{4})$ (Fig. 12). Any arbitrary symmetry operation can be depicted this way. For

Table 2
Crystallographic atom properties.

Property	Description
adpmax	The maximum anisotropic displacement parameter for the selected atom
adpmin	The minimum anisotropic displacement parameter for the selected atom
cell	Crystallographic unit cell, expressed either in lattice integer notation (111–999) or as a coordinate in *ijk* space; cell 555 equates to (1, 1, 1)
configuration	In the context `{configuration=n}` selects the *n*th disorder set
fx, *fy*, *fz*	Fractional coordinates along the *a*, *b* and *c* axes
fxyz	Fractional coordinates as a point (*fx*, *fy*, *fz*)
molecule	Molecule number
occupancy	CIF site occupancy
partialCharge	Partial charge
site	Crystallographic site number
symop	Symmetry operation code that generated this atom
symmetry	List of crystallographic symmetry operators generating this atom
temperature	Temperature factor (*B* factor)
ux, *uy*, *uz*	Normalized unit-cell coordinates along the *a*, *b* and *c* axes (all values between 0 and 1)
uxyz	Normalized unit-cell coordinates as a point (*ux*, *uy*, *uz*) (all values between 0 and 1)
x, *y*, *z*	Cartesian coordinates
xyz	Cartesian coordinates as a point (*x*, *y*, *z*)

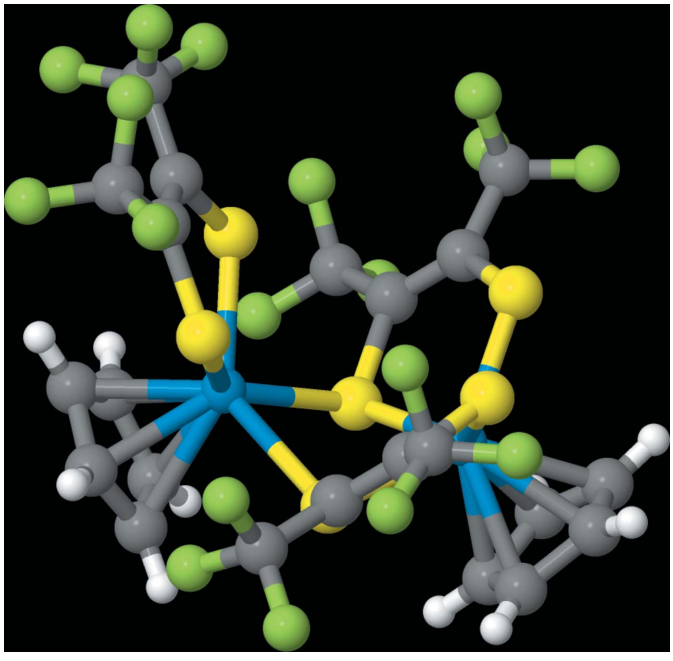

Figure 9
A tungsten complex, configuration 1. The selection of atoms is based on the value in the CIF atom site field _atom_site_disorder_group (`load 04369a.cif {2 1 1}; axes off; unitcell off; display configuration=1 and molecule=1`).

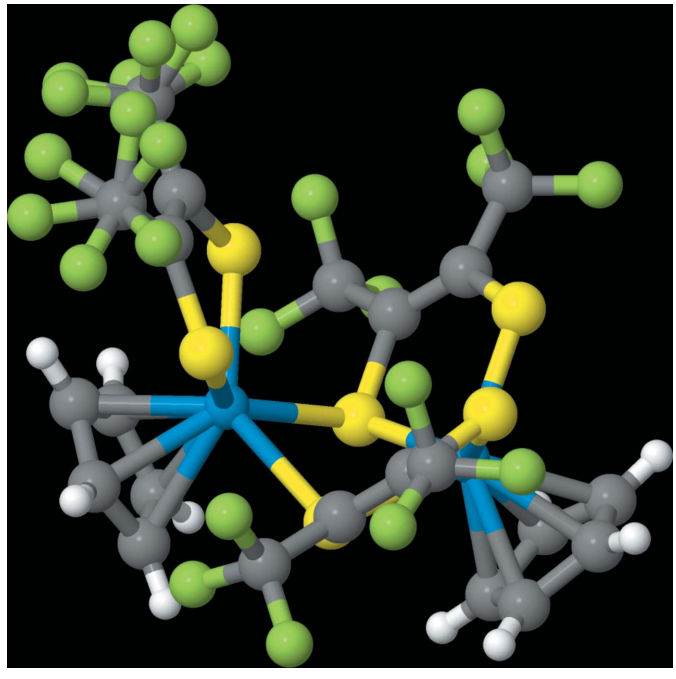

Figure 10
A superposition of two configurations (Miessler & Schaus, 2005). Disorder is evident in the methyl groups attached to one of the 1,2-ethenedithiolate ligands (`load 04369a.cif {2 1 1}; axes off; unitcell off; display molecule=1`).

example, opening a file with space group $P2_1/c$ and then using `draw symop "x,1/2-y,z+1/2"` will depict that *c*-glide plane operation.

In fact, if we knew that two molecules '1' and '4' were related in some way but we did not know how, we could find that out simply by using `show symop {molecule=1} {molecule=4}`. If more than one symmetry operation relates the two molecules, then both will be listed. Even better, if we wish to depict the symmetry operation, we just use `draw` instead of `show` (Fig. 13), and if we specify `set picking symmetry`, then the user can simply pick any two atoms, and *Jmol* will depict the symmetry relationship between them (Fig. 14).

Thus, *Jmol* can be used in a novel exploratory mode, where we are interested in checking out the sorts of relations between molecules or atoms in a crystal structure. A web page

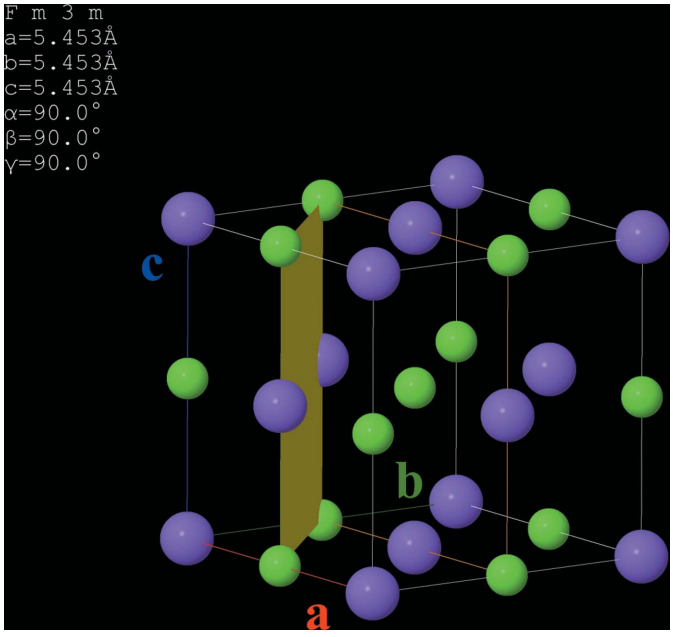

Figure 11
NaCl model showing two Miller planes (`load NaCl.cif packed; draw plane1 INTERSECTION unitcell hkl {2 2 0} color yellow; draw plane2 INTERSECTION unitcell hkl {0 2 0} color yellow mesh nofill`).

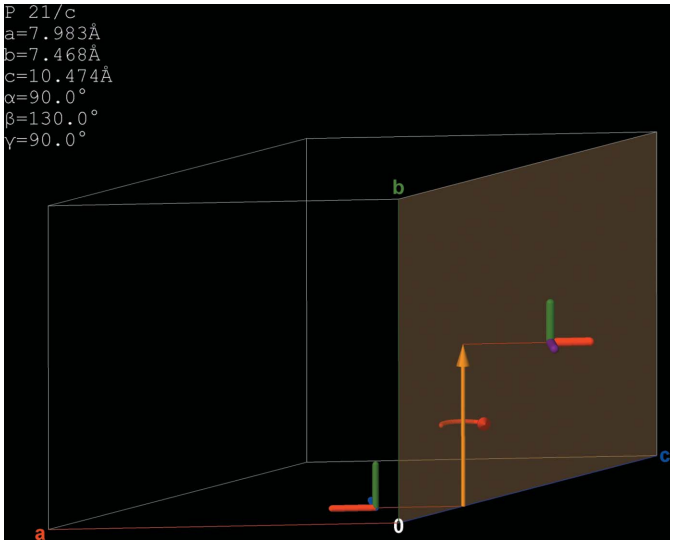

Figure 12
Crystal with space group $P2_1/c$, showing the operation of twofold screw axis $(-x, y + \frac{1}{2}, -z + \frac{1}{2})$ relating points $(\frac{1}{4}, 0, \frac{1}{4})$ and $(-\frac{1}{4}, \frac{1}{2}, \frac{1}{4})$ (`load maleic.cif 3; display none; draw symop 2 {1/4 0 1/4}`).

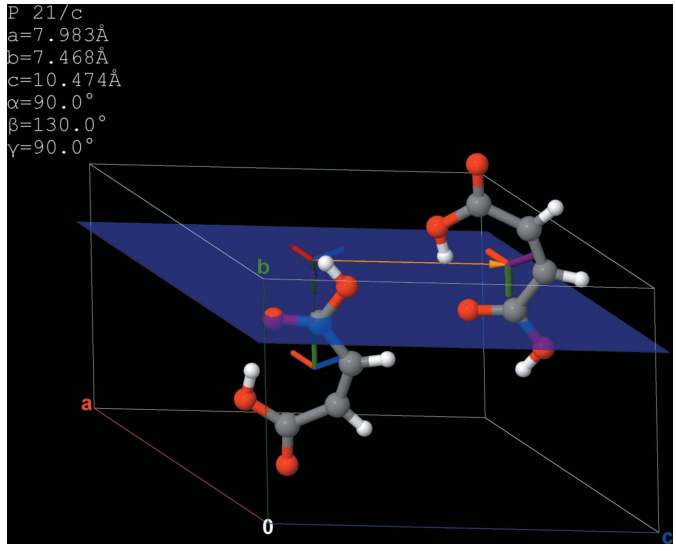

Figure 13
The *c*-glide plane operation $(x, \frac{3}{2} - y, z + \frac{1}{2})$ relating two molecules of maleic acid. The molecule on the left is being reflected through the plane, then translated by half a unit cell in the direction of the *c* axis (`load maleic.cif 3; display molecule=1 or molecule=4; draw symop {molecule=1} {molecule=4}`).

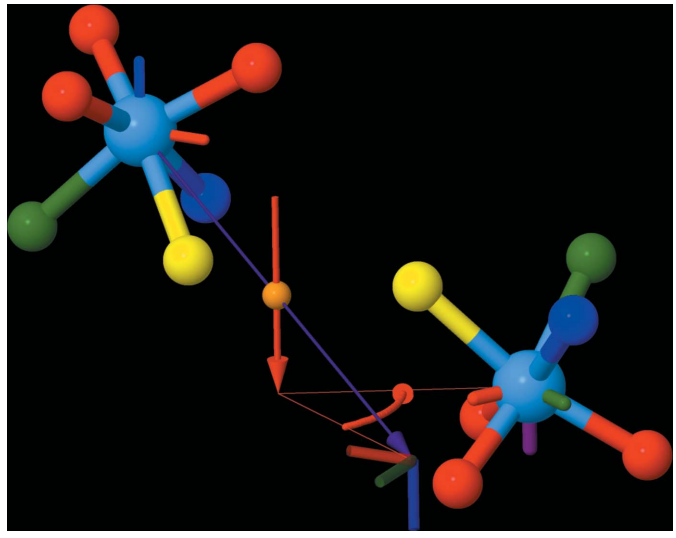

Figure 14
Using `set picking symmetry`, the user can click on any two atoms for a depiction of the symmetry operation that relates them. In this case, a $\bar{6}$ axis is involved [Wilkens & Mueller-Buschbaum, 1993; ICSD (http://icsd.Fiz-karlsruhe.de/icsd/) entry 73182]. The center on the left is inverted through a point, then rotated by 60° (`load icsd_73182.cif {2 1 1} packed; unitcell off; axes off; x = {atomno=5 or atomno=67}; display x or connected(x); draw symop {x}[1] {x}[2]`).

Table 3
All bonds connected to carbon.

```
$ print measure({_C}, {*}, "connected", "nm", "%0.3VALUE %UNITS\t%U1\t%U2")
```

0.145 nm	C5 #5	C3 #3
0.141 nm	C5 #5	N4 #4
0.125 nm	C5 #5	O11 #11
0.142 nm	C6 #6	N2 #2
0.142 nm	C6 #6	N4 #4
0.125 nm	C6 #6	O9 #9
0.139 nm	C7 #7	N2 #2
0.143 nm	C7 #7	C3 #3
0.140 nm	C7 #7	N21 #21
0.112 nm	C10 #10	H1 #1
0.144 nm	C10 #10	N4 #4
0.112 nm	C10 #10	H14 #14
0.112 nm	C10 #10	H15 #15
0.144 nm	C13 #13	N2 #2
0.112 nm	C13 #13	H16 #16
0.112 nm	C13 #13	H17 #17
0.112 nm	C13 #13	H18 #18
0.143 nm	C19 #19	N8 #8
0.112 nm	C19 #19	H22 #22
0.112 nm	C19 #19	H23 #23
0.113 nm	C19 #19	H24 #24
0.139 nm	C20 #20	N8 #8
0.110 nm	C20 #20	H12 #12
0.136 nm	C20 #20	N21 #21

illustrating these capabilities accompanies the publication of this paper (Hanson, 2009).

4.5. Measuring interatomic distances

One of the most common interests in crystallography is to measure interatomic distances and angles. With *Jmol*'s print command, again, this is almost trivial. To list all bond distances to C atoms, one uses `print measure({_C}, {*}, "connected")` (Table 3); to measure all close-contact non-hydrogen nonbonded distances we might issue `print measure({!_H}, {!_H}, 0, 1.5, "notconnected")`.

4.6. Mathematical scripting

One of the most powerful aspects of *Jmol* is its extensive mathematical scripting capability, which allows extensive analysis of structure. This is a relatively recent addition to *Jmol* and marks a major advance over the former minimal linear command-based scripting of *RasMol* and *Chime*. One can now use all of the popular command flow syntaxes common to modern programming languages, including if/else, for/next and while. *Jmol* allows for the creation of functions that augment the language in many ways. One can define variables of numerous types, including some more exotic types specifically useful in molecular structure analysis, for example planes, quaternions, axis-angles, atom and bond sets, and rotation matrices.

4.7. Callbacks to JavaScript

For a truly interactive experience one needs to build into a tutorial the possibility of feedback. Questions such as 'Where did the user click?', 'Has an atom been selected?' and 'Was the file loaded successfully?' are answered best by the mechanism of callback functions. These are JavaScript functions designed into the applet-containing web page that receive notices when events involving user actions (such as atom picking) or page actions (such as resizing) arise. *Jmol* allows for a number of callback notifications, including file-opening status, animation status, mouse clicking, atom picking and hovering, distance, angle and torsion measurement, script status, message reporting, and several others.

4.8. Database exploration

We recently wanted to ask a question about environments of amino acids and nucleic acids in the entire PDB. By writing a simple *Jmol* script and running *Jmol* as a stand-alone application, we could compile data on all of the proteins and nucleic acids (or, actually, a certain subset of well characterized structures). While *Jmol* may not be the most efficient means of doing this sort of analysis, the power of *Jmol*'s scripting language made the task quite simple. Just about any aspect of biomolecular structure can be investigated this way.

In our case, we were interested in a property we have recently discovered, quaternion-based straightness (Hanson *et al.*, 2010). Fundamentally, this property measures relative orientation of groups within a model. In general, we expect straightness to be high within secondary structures such as helices and sheets and low in less structurally defined regions. One of the DNA–protein complexes investigated, however, was found to have very low straightness within its helix (Fig. 15). Upon closer inspection, it was found that one of the

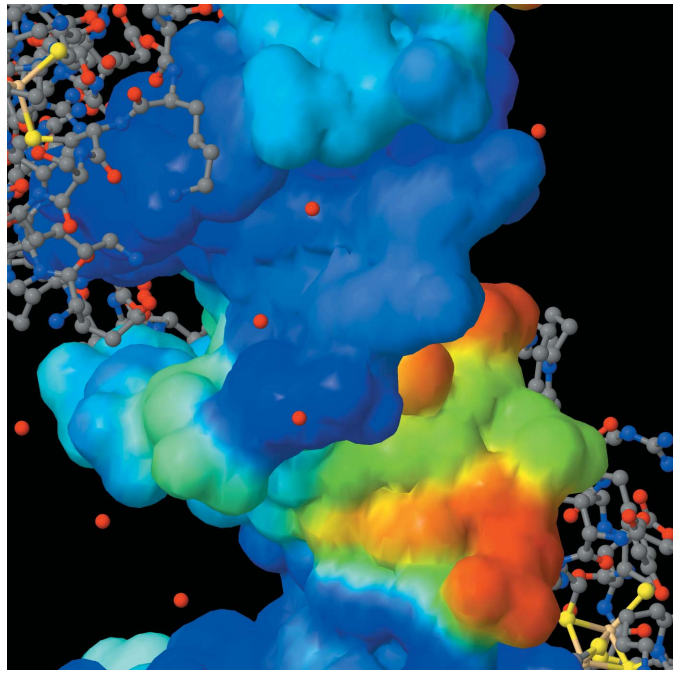

Figure 15
A portion of a DNA–protein complex (PDB code 1d66; Marmorstein *et al.*, 1992) with the DNA van der Waals surface colored by relative orientation of bases. The sharp coloration change in the center right indicates a region of unusually low straightness (`load =1d66; set quaternionFrame "C"; isosurface select(DNA) ignore(not DNA) vdw map property straightness`).

cytidine bases was flipped (Fig. 16). Upon communication with the author of the original study, it was found that a mistake in the model used for the crystallographic analysis was involved.

From an educational point of view, this example simply illustrates that the models we find in the PDB database should not be taken at face value and how programs like *Jmol* can be used to explore databases and to spot both expected and unexpected structural patterns.

4.9. Program output

Largely based on user requests, *Jmol* has an extensive suite of output options that complement its interactive use. With either the stand-alone version or the signed applet one can write files to disk or to the operating system clipboard and produce high-quality images or exported models. The most popular image-creation options – JPG and PNG – are fully supported. In addition, while *Jmol*'s output quality is very high, even higher 'point-of-view ray tracing' (*POV-Ray*, 2000) output is as simple as clicking a button on the tool bar of the application or selecting a menu option on the applet.

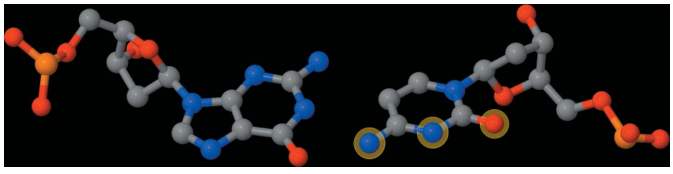

Figure 16
Closer inspection of the CG base pair in Fig. 15 shows an anomalously flipped cytidine (on the right). The three highlighted atoms should be aligned with the guanidine.

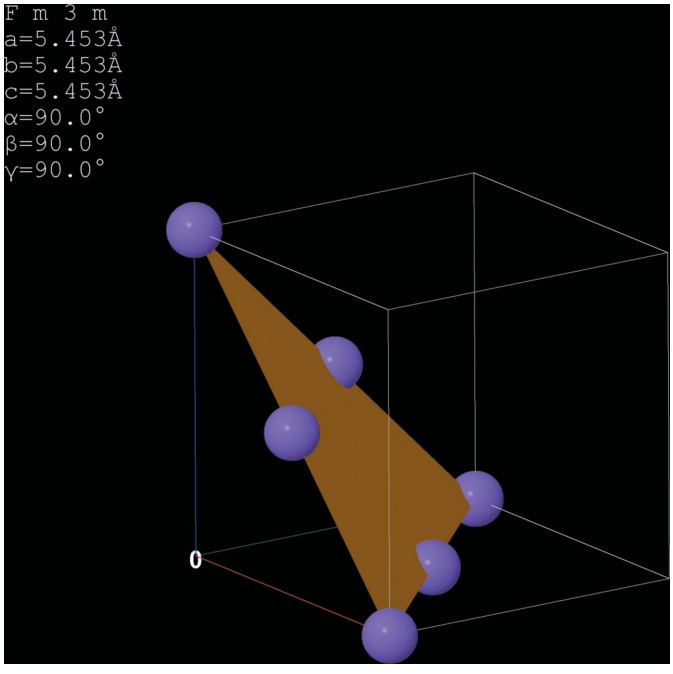

Figure 17
NaCl model depicting the (111) Miller plane and associated atoms (`load NaCl.cif packed; display within(0, hkl, {1 1 1}); draw intersection unitcell hkl {1 1 1}`).

One of the interesting aspects of these two-dimensional image files is that they can be read back into *Jmol* to reproduce the exact three-dimensional scene depicted in the image. The almost magical quality of this dramatic result is always a hit with students in the classroom.

Finally, *Jmol* can also export models in a variety of formats readable by other three-dimensional visualization programs.

4.10. Surface generation and property mapping

An important aspect of crystallography involves the visualization of lattice planes specified with Miller indices. *Jmol* allows selection and display of atoms based on their proximity to Miller planes. So, for example, in NaCl, space group $Fm\bar{3}m$, one can first depict the (111) Miller plane using `draw INTERSECTION unitcell hkl {1 1 1}` and then display just the atoms on that plane using `display within(0, hkl, {1 1 1})` (Fig. 17). The zero here indicates that we want atoms on the plane; a positive or negative number instead would select atoms within the specified distance on one side (positive) or the other (negative) of the plane. Since the Miller plane represents just one in an infinite family of planes, *Jmol* allows depiction of any member of this family by simply scaling the integers to the desired value: $(\frac{222}{333})$, for example. An interesting effect is to create a surface that maps atom position onto a plane. This is done using `isosurface hkl {2/3 2/3 2/3} map molecular`. These maps roughly approximate the look of a slice of electron density (Fig. 18).

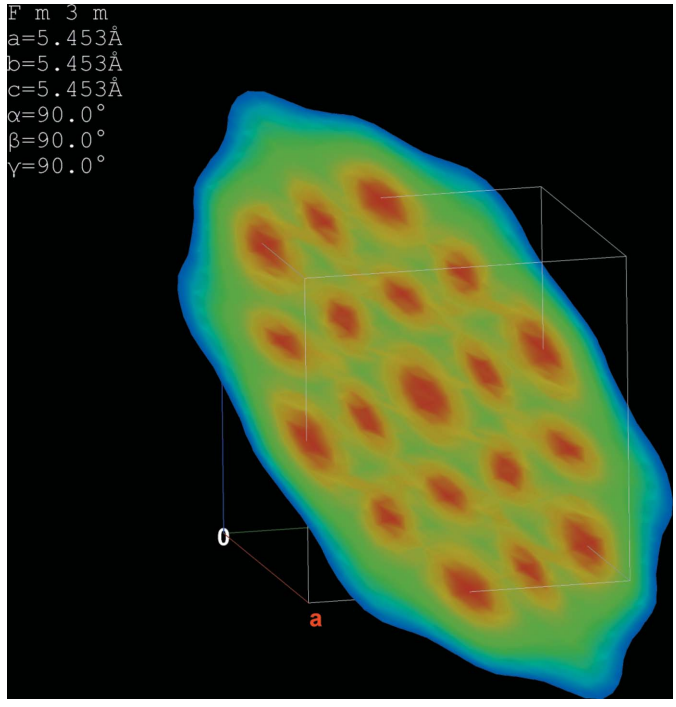

Figure 18
Surface through a plane parallel to the (111) Miller plane highlighting atom positions. This depiction can highlight symmetry within any arbitrary plane (`load NaCl.cif packed; display none; isosurface hkl {2/3 2/3 2/3} map molecular`).

4.11. Novel depictions of electron density

One of the foremost challenges of instructors is giving students a sense of what a 'structural model' actually is and how we arrive at that model from actual data. The textbook view – of balls and sticks and cartoonish helices and sheets – properly conveys neither the ambiguity of structure nor the mathematical origins of structural models. With the availability of online electron density servers such as the Uppsala Electron Density Server (*EDS*, 2010), *Jmol* can be used to help develop an appreciation for the underlying mathematical model from which these more common renderings derive. *Jmol* can depict standard mesh-type isosurfaces of electron density, but in addition, *Jmol* can represent electron-density maps using a grid-based 'cloud' method. With this method, one can depict the three-dimensional grid of electron-density data in its raw form as a block of numbers, in which some hint of 'structure' is present (Fig. 19). The simple act of progressively removing numbers from this block based on a cut-off value 'reveals' the underlying structure as a sort of pointillist model in a novel and very striking manner that does not rely on the more abstract concept of an isosurface (Fig. 20). The experience of 'discovering' the structure within the data is dramatic (*DensitySlider*, 2010).

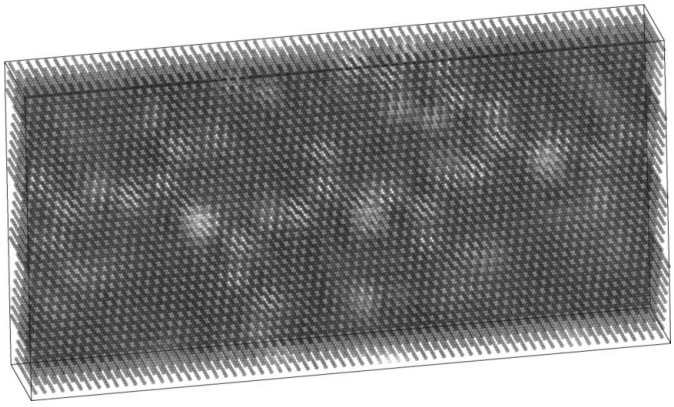

Figure 19
Electron density as a cloud for 3hyd (Ivanova *et al.*, 2009; CCP4 map file http://eds.bmc.uu.se/cgi-bin/eds/uusfs?pdbCode=3hyd). Each point represents one data point in the map file, with opacity scaled relative to calculated electron density. It is clear that *something* is there, but what that might be is not at all clear. *Jmol* command: `load =3HYD; boundbox on; background white; isosurface boundbox color density cutoff 0 "=3HYD" colorScheme translucent BW`.

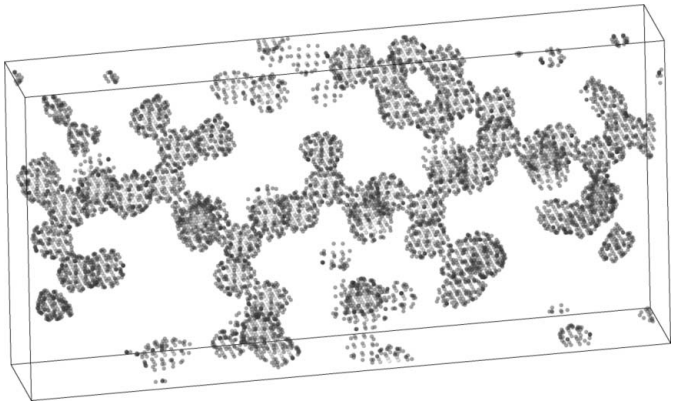

Figure 20
Electron density as a cloud (3hyd, cutoff 1.6 e Å^{-3} or σ = 1.0). Simply by eliminating data points with values below a specified cut-off value, the structure of the protein backbone and, among others, a tyrosine side chain (top center) emerges. The surface enclosing these points would be the commonly drawn isosurface associated with a standard electron-density map.

4.12. Depicting uncertainty and dynamics

A major challenge in early crystallographic education is helping students to develop an understanding of the uncertainties inherent in models. *Jmol* can, of course, depict uncertainty in the standard form of displacement ellipsoids, but in addition to that, *Jmol* can depict isotropic *B*-value ('temperature') data found in PDB and mmCIF formats in numerous ways. For example, one can map isotropic temperature data onto a molecular surface (Fig. 21) or depict *B* factors as the radius of a sphere at a given atom position (Fig. 22). In addition, *Jmol* can read and animate the results of molecular dynamics calculations, thus simulating the range of natural molecular motion at a given temperature.

5. Summary

Jmol is a versatile tool that can readily enhance many discussions relating to crystallography by aiding in the visualization of real crystallographic data in both traditional and nontraditional ways. With its extremely flexible file-loading and symmetry-handling capabilities, *Jmol* can be used to

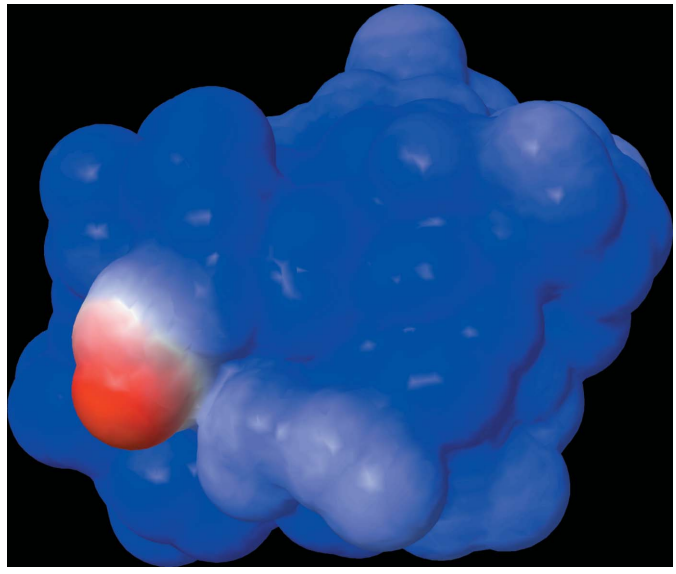

Figure 21
Temperature (*B*-factor) data mapped onto a molecular surface for 1crn (Teeter, 1984). Red indicates residues having the highest *B* factor (blue lowest). Any sort of atom-based data can be mapped onto an isosurface in this way (`load =1crn; isosurface molecular map property temperature colorScheme bwr`).

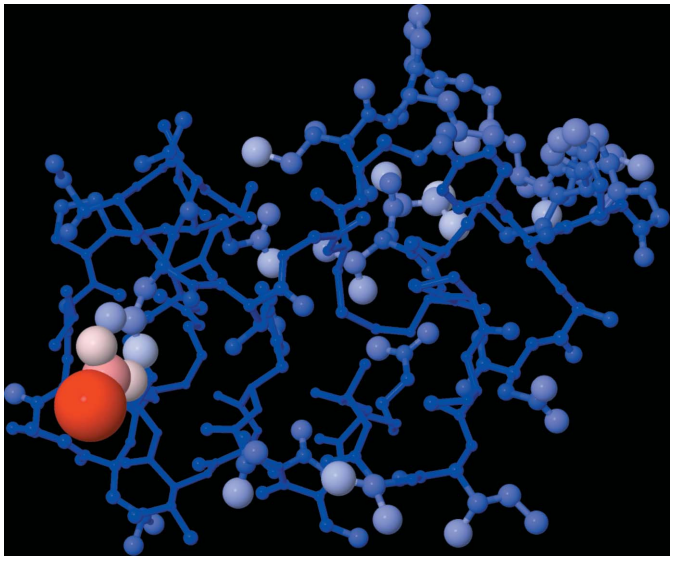

Figure 22
Temperature data depicted as spheres of different size and color – an alternative to the standard mapping shown in Fig. 21. In this depiction, larger spheres indicate higher positional uncertainty in the data set (`load =1crn; {*}.radius={*}.temperature.all.mul(0.05); color temperature`).

highlight the essential characteristics of unit cells, space groups and symmetry operators. Its rich mathematical scripting language and close connection to JavaScript allows detailed exploration and 'guided tours' of systems of interest and has allowed database developers the unprecedented capability to produce highly customized visual front ends for their products. It behoves us as educators to introduce our students to these database resources and to emphasize a critical-thinking approach to their use: Is this model reasonable? What is its origin? What assumptions did the authors make? What are the uncertainties? These are the sorts of questions that students need to be thinking about, and while many of them are outside the scope of *Jmol*, many at least initially can be addressed using visualization.

Science education is all about communication – teachers communicating complex molecular interactions and symmetry relationships; students making presentations and learning from web-based tutorials and quizzes. As the technology of visualization has become more prevalent and expected, *Jmol* has proven to be a solid and dependable partner in project after project at all levels of the educational enterprise.

Communication, of course, is all about *community*, and this is where *Jmol* has made a unique and lasting contribution to education. The features discussed in this paper are not the isolated invention of a lone programmer or even that of a small developer team or research group. Rather, these features are the result of a whole new 21st-century way of doing business, incorporating peer-reviewed solutions based on ideas generated within an active user community of professional crystallographers, educators and students with turnaround times of hours to days rather than months to years.

In all, the focus in this paper has been on the features of *Jmol* that might be particularly useful in an educational setting. As with all such tools, it is really the creativity of the user, not the programmer, that defines the end result, and while many examples of *Jmol*'s use in molecular structure education are available (JmolWiki, 2010), far more is possible than has been realized to date. By itself on a web page, *Jmol* is just a fantastically powerful black box. What makes it so useful is how easy it is to turn that black box into an interactive and educational window into the beauty of the molecular world.

It is not possible to thank all of the people who have made contributions to the *Jmol* project. Dan Gezelter was the original developer of *Jmol*, to whom we are all very much indebted. Several other programmers contributed over the years, most notably Egon Willighagen, Nico Vervelle, René Kanters and especially Michael (Miguel) Howard, who single-handedly made *Jmol*'s rendering engine a marvel of Java programming. Many *Jmol* users have contributed ideas, designs and solutions to problems over the years. Special thanks go to Tim Driscoll, Frieda Reichsman, Angel Herráez, Brian McMahon, Peter Murray-Rust, Alan Hewat and Sydney Hall, among many, many others. An undergraduate in our research group, Dan Kohler, discovered the optimal definition of straightness and found the anomaly in PDB entry 1d66.

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