Visualization of Fundamental Symmetries in Nature

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Abstract: Most matter in nature and technology is composed of crystals and crystal grains. A full understanding of the inherent symmetry is vital. A new interactive software tool is demonstrated, that visualizes 3D space group symmetries. The software computes with Clifford (geometric) algebra. The space group visualizer (SGV) is a script for the open source visual CLUCalc, which fully supports geometric algebra computation. In our presentation we will first give some insights into the geometric algebra description of space groups. The symmetry generation data are stored in an XML file, which is read by a special CLUScript in order to generate the visualization. Then we will use the Space Group Visualizer to demonstrate space group selection and give a short interactive computer graphics presentation on how reflections combine to generate all 230 three-dimensional space groups.

1 Introduction

Crystals are fundamentally periodic geometric arrangements of molecules. The directed distance between two such elements is a Euclidean vector in $\mathbb{R}^3$. Intuitively all symmetry properties of crystals depend on these vectors. Indeed, the geometric product of vectors [8] combined with the conformal model of 3D Euclidean space [5, 9, 15, 16, 25] yield an algebra fully expressing crystal point and space groups [10, 13, 14, 18]. Two successive reflections at (non-) parallel planes express (rotations) translations, etc. [6, 7]. This leads to a 1:1 correspondence of geometric objects and symmetry operators with vectors and their products (Lipschitz elements, called *versors* in [13]), ideal for creating a suit of interactive visualizations using CLUCalc [1, 2] and OpenGL [18].

Excellent modern introductions to geometric algebra are [2–4].

In this work we used CLUCalc [1, 2], a freely available software tool for 3D visualizations and scientific calculations that was conceived and written by C. Perwass. CLUCalc interprets a script language called *CLUScript*, which has been designed to make mathematical calculations and visualizations very intuitive. Currently CLUViz Home 5.1 is only available for Windows XP/Vista. The installation file of CLUViz Home 5.1 can be freely downloaded and installed. The software package comes with a manual and many examples. The CLUViz Home edition is free for non-commercial use.

Some of the main CLUViz features are: Easy creation of interactive visualizations for geometry, physics, human machine interfaces, image processing and more. Direct programming of shaders from within CLUScripts using the OpenGL shading language, for image processing and fast mathematical calculations. It is possible to run CLUViz visualizations from within other `C++` or `C#` programs using the CLUViz or CLUVizNET DLL.

The latest (2009) of CLUCalc is contained in the visualization suite CLUViz. CLUViz separates the visualization engine from the CLUScript editor CLUCalc. Therefore one can now use the visualization power of CLUCalc from within other `C++` and `C#` programs. The CLUViz distribution also includes the editor CLUCalc.

The older version CLUCalc v4.3.3 is still available as binaries and source code. CLUViz 5.1 is only available as Windows binary, so far.

Before describing the actual visualization, we briefly introduce some notions from Clifford geometric algebra (GA) and the GA description of crystal symmetry.

2 Clifford's geometric algebra

Clifford's associative geometric product [8] of two vectors simply adds the inner product to the outer product of Grassmann

$$\vec{a}\vec{b} = \vec{a} \cdot \vec{b} + \vec{a} \wedge \vec{b}. \tag{1}$$

Under this product parallel vectors commute and perpendicular vectors anti-commute

$$\vec{a}\vec{x}_{\parallel} = \vec{x}_{\parallel}\vec{a}, \qquad \vec{a}\vec{x}_{\perp} = -\vec{x}_{\perp}\vec{a}. \tag{2}$$

This allows to write the reflection of a vector $\vec{x}$ at a hyperplane through the origin with normal $\vec{a}$ as

$$\vec{x}\,' = -\,\vec{a}^{\,-1}\vec{x}\,\vec{a}, \qquad \vec{a}^{\,-1} = \frac{\vec{a}}{\vec{a}^{\,2}}. \tag{3}$$

The composition of two reflections at hyperplanes whose normal vectors $\vec{a}, \vec{b}$ subtend the angle $\alpha/2$ yields a rotation around the intersection of the two hyperplanes by α

$$\vec{x}\,' = (\vec{a}\vec{b})^{-1}\vec{x}\,\vec{a}\vec{b}, \qquad (\vec{a}\vec{b})^{-1} = \vec{b}^{\,-1}\,\vec{a}^{\,-1}. \tag{4}$$

Continuing with a third reflection at a hyperplane with normal $\vec{c}$ according to Cartan yields rotary reflections and inversions

$$\begin{aligned} \vec{x}\,' &= -\,(\vec{a}\vec{b}\vec{c})^{-1}\vec{x}\,\vec{a}\vec{b}\vec{c}, \\ \vec{x}\,'' &= -\,i^{-1}\vec{x}\,i, \\ i &\doteq \vec{a} \wedge \vec{b} \wedge \vec{c}, \end{aligned} \tag{5}$$

where $\doteq$ means equality up to non-zero scalar factors (which cancel out in (6)). In general the geometric product of k normal vectors (the versor S) corresponds to the composition of reflections to all symmetry transformations [13] of 2D and 3D crystal cell point groups

$$\vec{x}\,' = (-1)^k S^{-1}\,\vec{x}\,S. \tag{6}$$

Table 1: Geometric (geom.) and international (int.) notation for 2D point groups.

Crystal	Oblique		Rectangular		Trigonal		Square Square		Hexagonal	
geo.	$\bar{1}$	$\bar{2}$	1	2	3	$\bar{3}$	4	$\bar{4}$	6	$\bar{6}$
int.	1	2	m	mm	3m	3	4m	4	6m	6

Table 2: Geometric 3D point group symbols (Symb.) [13] and generators (Gen.) with $\theta_{\vec{a},\vec{b}} = \pi/p$, $\theta_{\vec{b},\vec{c}} = \pi/q$, $\theta_{\vec{a},\vec{c}} = \pi/2$, $p, q \in \{1, 2, 3, 4, 6\}$.

Symb.	p	$\bar{p}$	pq	$\bar{p}q$	$p\bar{q}$	$\bar{p}\bar{q}$	$\overline{pq}$
Gen.	$\vec{a}, \vec{b}$	$\vec{a}\vec{b}$	$\vec{a}, \vec{b}, \vec{c}$	$\vec{a}\vec{b}, \vec{c}$	$\vec{a}, \vec{b}\vec{c}$	$\vec{a}\vec{b}, \vec{b}\vec{c}$	$\vec{a}\vec{b}\vec{c}$

3 Geometric algebra description of crystal symmetry

3.1 Two dimensional point groups

The 10 2D point groups (2D crystal classes) [13] are generated by multiplying vectors selected [18] as in Fig. 1. The index p can be used to denote these groups as in Table 1. For example the hexagonal point group is given by multiplying its two generating vectors $\vec{a}, \vec{b}$

$$6 = \{\vec{a}, \vec{b}, R = \vec{a}\vec{b}, R^2, R^3, R^4, R^5, R^6 = -1,$$
$$\vec{a}R^2, \vec{b}R^2, \vec{a}R^4, \vec{b}R^4\}. \quad (7)$$

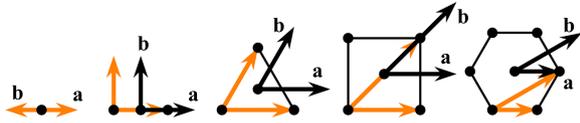The rotation subgroups are denoted with bars, e.g. $\bar{6}$.

Figure 1: Regular polygons ($p = 1, 2, 3, 4, 6$) and point group generating vectors $\vec{a}, \vec{b}$ subtending angles π/p shifted to center.

3.2 Three dimensional point groups

The selection of three vectors $\vec{a}, \vec{b}, \vec{c}$ from each crystal cell [13, 18] for generating all 3D point groups (3D crystal classes) is indicated in Fig. 2. Using $\angle(\vec{a}, \vec{b})$ and $\angle(\vec{b}, \vec{c})$ we can denote all 32 3D point groups as in Table 2. For example the monoclinic point groups are then (int. symbols: 2/m, m and 2, respectively)

$$2\bar{2} = \{\vec{c}, R = \vec{a} \wedge \vec{b} = i\vec{c}, i = cR, 1\},$$
$$1 = \{\vec{c}, 1\}, \quad \bar{2} = \{i\vec{c}, 1\}. \quad (8)$$

3.3 Space groups

The smooth composition with translations is best done in the conformal model [5, 9, 15–17, 25] of Euclidean
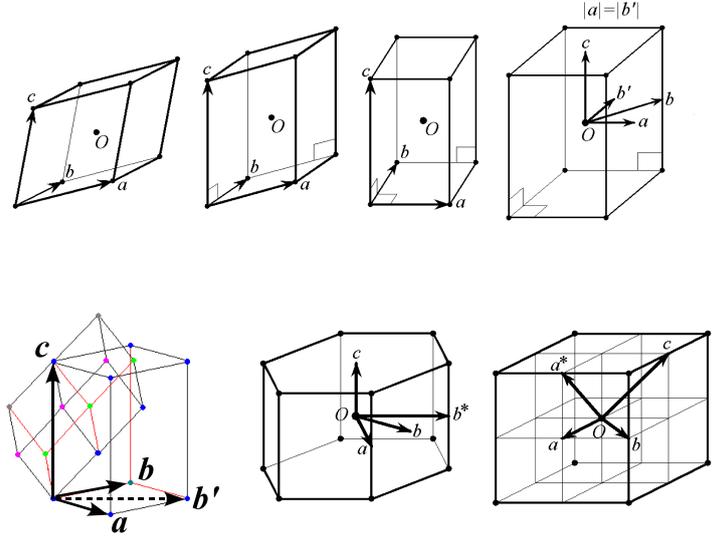

Figure 2: 7 crystal cells with vector generators $\vec{a}, \vec{b}, \vec{c}$: triclinic, monoclinic, orthorhombic, tetragonal, trigonal (rhombohedral), hexagonal, cubic.

space (in the GA of $\mathbb{R}^{4,1}$), which adds two null-vector dimensions for the origin $\vec{e}_0$ and infinity $\vec{e}_\infty$

$$X = \vec{x} + \frac{1}{2}\vec{x}^2\vec{e}_\infty + \vec{e}_0,$$
$$\vec{e}_0^2 = \vec{e}_\infty^2 = X^2 = 0, \quad (9)$$
$$X \cdot \vec{e}_\infty = -1.$$

The inner product of two conformal points gives their Euclidean distance and therefore a plane m equidistant from two points A, B as

$$X \cdot A = -\frac{1}{2}(\vec{x} - \vec{a})^2 \Rightarrow X \cdot (A - B) = 0,$$
$$m = A - B \propto \vec{p} - d\vec{e}_\infty, \quad (10)$$

where $\vec{p}$ is a unit normal to the plane and d its signed scalar distance from the origin. Reflecting at two parallel planes m, m' with distance $\vec{t}/2$ we get the *translat*ion opera*tor* (by $\vec{t}$)

$$X' = m'm\,X\,mm' = T_{\vec{t}}^{-1}XT_{\vec{t}}, \quad T_{\vec{t}} = 1 + \frac{1}{2}\vec{t}\vec{e}_\infty. \quad (11)$$

Reflection at two non-parallel planes m, m' yields the rotation around the m, m'-intersection by twice the angle subtended by m, m'.

Group theoretically the conformal group $C(3)$ is isomorphic to $O(4, 1)$ and the Euclidean group $E(3)$ is the subgroup of $O(4, 1)$ leaving infinity $\vec{e}_\infty$ invariant [13]. Now general translations and rotations are represented by geometric products of vectors (Lipschitz elements, called versors in [13]). To study combinations of versors it is useful to know that (cf. Table 3)

$$T_{\vec{t}}\vec{a} = \vec{a}T_{\vec{t}'}, \qquad \vec{t}' = -\vec{a}^{-1}\vec{t}\vec{a}. \quad (12)$$

Applying these techniques one can compactly tabulate geometric space group symbols and generators [13]. Table 4 implements this for the 13 monoclinic space groups. All this is interactively visualized by the Space Group Visualizer [18–24].

Table 3: Computing with reflections and translations. The vectors $\vec{a}, \vec{b}$ are pictured in Fig. 1.

$\angle(\vec{a},\vec{b})$	180°	90°	60°	45°	30°
$T_{\vec{a}}\,\vec{b} =$	$\vec{b}\,T_{-\vec{a}}$	$\vec{b}\,T_{\vec{a}}$	$\vec{b}\,T_{\vec{a}-\vec{b}}$	$\vec{b}\,T_{\vec{a}-\vec{b}}$	$\vec{b}\,T_{\vec{a}-\vec{b}}$
$T_{\vec{b}}\,\vec{a} =$	$\vec{a}\,T_{-\vec{b}}$	$\vec{a}\,T_{\vec{b}}$	$\vec{a}\,T_{\vec{b}-\vec{a}}$	$\vec{a}\,T_{\vec{b}-2\vec{a}}$	$\vec{a}\,T_{\vec{b}-3\vec{a}}$

Table 4: Monoclinic space group versor (Lipschitz element) generators (gen.), $T^A = T_{\vec{b}+\vec{c}}^{1/2}$, int. = international name [11] in col. 2, # = Int. # in col. 1, geo. = geometric name in col. 3, alt. = alternative, columns 3 and 4: [13]. $T_{\vec{a}}, T_{\vec{b}}, T_{\vec{c}}$ suppressed.

#	Int.	Geo.	Geo. gen.	Int. gen.	Alt. gen.
3	$P2$	$P\bar{2}$	$i\vec{c} = \vec{a} \wedge \vec{b}$		
4	$P2_1$	$P\bar{2}_1$	$i\vec{c}T_{\vec{c}}^{1/2}$		
5	$C2$	$A\bar{2}$	$i\vec{c}$, T^A		
6	Pm	$P1$	$\vec{c}$		
7	Pc	P_a1	$\vec{c}T_{\vec{a}}^{1/2}$		
8	Cm	$A1$	$\vec{c}$, T^A		
9	Cc	A_a1	$\vec{c}T_{\vec{a}}^{1/2}$, T^A		
10	$P2/m$	$P2\bar{2}$	$\vec{c}$, $i\vec{c}$	i, $i\vec{c}$	i, $\vec{c}$
11	$P2_1/m$	$P2\bar{2}_1$	$\vec{c}$, $i\vec{c}T_{\vec{c}}^{1/2}$	i, $i\vec{c}T_{\vec{c}}^{1/2}$	i, $\vec{c}T_{\vec{c}}^{1/2}$
12	$C2/m$	$A2\bar{2}$	$\vec{c}$, $i\vec{c}$, T^A	iT^A, $i\vec{c}T^A, T^A$	i, $\vec{c}$, T^A
13	$P2/c$	$P_a2\bar{2}$	$\vec{c}T_{\vec{a}}^{1/2}$, $i\vec{c}$	i, $i\vec{c}T_{\vec{a}}^{1/2}$	i, $\vec{c}T_{\vec{a}}^{1/2}$
14	$P2_1/c$	$P_a2\bar{2}_1$	$\vec{c}T_{\vec{a}}^{1/2}$, $i\vec{c}T_{\vec{c}}^{1/2}$	i, $i\vec{c}T_{\vec{a}+\vec{c}}^{1/2}$	i, $\vec{c}T_{\vec{a}+\vec{c}}^{1/2}$
15	$C2/c$	$A_a2\bar{2}$	$\vec{c}T_{\vec{a}}^{1/2}$, $i\vec{c}$, T^A	i, $i\vec{c}T_{\vec{a}}^{1/2}, T^A$	i, $\vec{c}T_{\vec{a}}^{1/2}, T^A$

4 Interactive Software Implementation

The realization in software relies on the visual multivector software CLUCalc (www.CLUCalc.info). The excellent graphics rendering is based on OpenGL graphics. The space group symmetry definitions described in the previous sections are denoted for each space group in the form of an XML input file. The XML files serve as input for a CLUCalc script named Space Group Visualizer (SGV).

4.1 The Space Group Visualizer GUI

Fig. 3 shows the SGV GUI. The SGV toolbar is magnified and annotated in Fig. 4. Depending on the displayed space group, basis vector lengths and (or) angles may not be changed. This is indicated by toolbar elements shown in gray.

4.2 Space group and symmetry selection

Figure 5 shows the interactive (hyperlink like) space group selection. Clicking blue text elements in the browser panel on the left of the GUI allows to access crystal systems, classes (point groups), and individual space groups.

Figure 6 illustrates the selection of symmetries from the complete list of *Symmetries* (left SGV GUI browser panel), which are present in the currently selected space group. Symmetries that are to be dis-
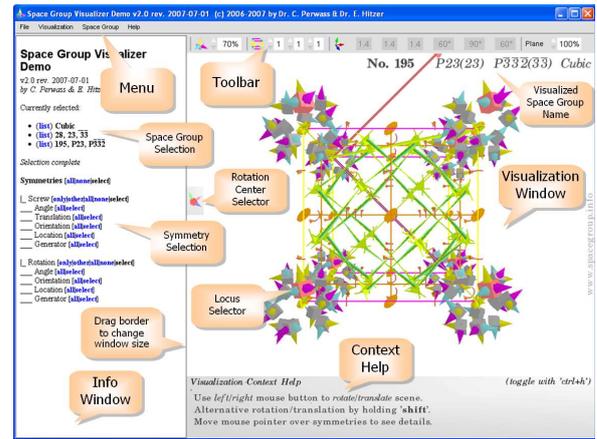

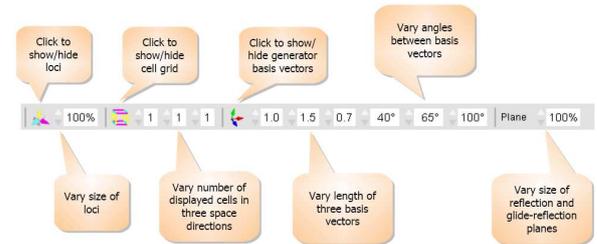Figure 3: GUI of the Space Group Visualizer.

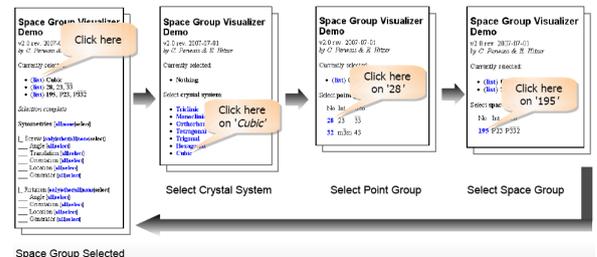Figure 4: Toolbar of the Space Group Visualizer.

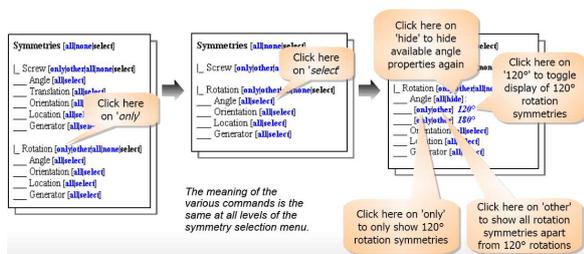Figure 5: Space group selection from the Space Group Visualizer browser panel.

Figure 6: Space group selection of individual symmetries or groups of symmetries to be displayed.

played can be selected according to their properties (angle, orientation, location, translation component). Several properties selected together will display only those symmetries that satisfy all properties. Another way is to open the generator list of a certain type of symmetry and select individual geometric algebra generators to be displayed (or to be removed from the display).

4.3   Mouse pointer interactivity

The mouse pointer allows a variety of visual interactions and animations, depending over which part of the visualization it is placed. Moving the mouse pointer over a symmetry element visualization both animates the symmetry and displays detailed information about this symmetry group element in the lower right corner. Animation means dynamic color and size changes; and the motion of general elements along a trajectory tracing the symmetry operation incrementally. Placement of the mouse pointer over a general element (locus) selector activates it (blinking). The mouse pointer over the rotation center selector allows to change the rotation center of the mouse activated view rotation (described below).

The mouse pointer can be placed anywhere inside the visualization window. Holding down the left (right) mouse button and moving the mouse will rotate (translate) the visualization. Alternative rotation axes (translation directions) are activated by additionally holding the SHIFT key. With a 3D-mouse (3dconnexion) one can rotate and translate the view along all axes simultaneously. First placing the mouse pointer over a general element (locus) selector permits to translate and rotate it (together with all its symmetric partners). This provides an excellent way to grasp how one general element and the 3D symmetry represented in the space group determine the whole crystal structure.

A special feature of the SGV is the direct 3D graphics interaction. Simply placing the mouse pointer over a symmetry activates it and allows to:

- Select only the activated symmetry (left mouse button). All other symmetries disappear from the view.

- Holding the CTRL key at the same time (while pressing the left mouse button) shows all symmetries (and only these) of the same type.

- Clicking the right mouse button removes an activated symmetry from the view.

- Holding the CTRL key at the same time (while pressing the right mouse button) removes all symmetries of the same type.

4.4   Visualization options in detail

The visualization drop down menu allows to toggle (activate and deactivate) the following visual functions

- Full screen mode.

- Orthographic view. The orthographic view allows the most direct comparison with ITA orthographic projections [11].

- Animation of the origin locus when a symmetry is activated (animated).

- Rotation animation of the whole view when it is *pushed* with the (left) mouse button.

- Reset the crystal view to visualizer default values.

- Reset general element (loci) positions.

The special visualization lighting menu provides a relative position light source. It is positioned relative to the visualization coordinate frame and moves with the visualization. Deselecting this option fixes the light source relative to the observer. The light source can optionally be positioned at the center of the coordinate frame, which is relative (or absolute) depending on the (de)selection of the relative position option. The ambient light submenu allows to adjust the brightness of the ambient light, leading to more dramatic effects for darker settings.

The color scheme menu item allows to select the current color scheme. For example a scheme with black background is more suitable for use in presentations, while a white background is better for publications, etc. It is possible via an XML file to individually define further color schemes. A color stereo option allows to specify cinema type stereo colors, which are best viewed with corresponding cinema color glasses in order to obtain the full spatial 3D effect akin to virtual reality.

The cell type menu allows to select between different cell choices in the IT, Volume A [11], and (if different) a special geometric algebra type cell, which has the generating vectors $\vec{a}, \vec{b}, \vec{c}$ as cell axis attached to the cell origin.

4.5   Integration with the online International Tables of Crystallography

Through the window menu an additional window can be opened for displaying the pages of a space group from the online version of the International Tables of Crystallography, Volume A (ITA) [11]. For this the
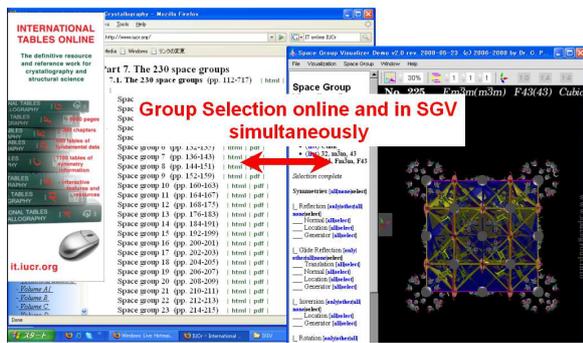
Figure 7: Parallel space group selection in the SGV window and the online ITA [11] space group window.

user must hold a valid user ID and password. When the online ITA can be accessed, the SGV and the online ITA window will always show the *same* space group. The user can synchronously navigate from space group to space group either in the SGV or in the online ITA window (cf. Fig. 7).

4.6 Saving results

It often takes some time to interactively bring the visualization into a desired state, which includes selection of a space group, selection and deselection of symmetry elements, 3D translations and rotations, adjustments of size, color and lighting, etc. If the user wants to save his work in order to show it to others, use it for teaching and presentations, produce publications, images for the internet, etc. the File menu offers the options to do a one step Quick Save View or a more detailed Save View. The latter will open a popup menu in order to choose the destination folder and the desired file name and file format. File formats available are: PNG (default), JPEG, Bitmap, Postscript, JPEG + EPS (get the same picture at once in two formats), and PNG with Bounding Box. The EPS option is particularly useful for use with Latex. In this way most of the figures were produced in this paper.

5   Conclusion

We have briefly reviewed the geometric algebra representation of $\mathbb{R}^3$ in the socalled conformal model and its use for the representation of 2D and 3D point groups and space groups. The key point is to only use physical crystal lattice vectors for the group generation. The second part introduced the interactive software visualization of 3D space group symmetries based on the established geometric algebra representation. This implementation uses the conformal model both for generating the graphics itself and for internally computing with space group transformations.

Future options are the visualization of extraordinary space group orbits, subperiodic space groups, and magnetic space groups. The latter seems particularly attractive as it may nicely integrate the bivector representation of spin [12] in the real Dirac-Hestenes equation of relativistic quantum physics. Based

on CLUCalc a first rudimentary geometric algebra protein visualizer has been programmed recently for proteins of several thousand (up to 10 000) atoms. A possible future molecule (or ion group) toolbox may therefore be able to display complex biomolecule crystals as well.

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