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THE SPACE GROUP VISUALIZER

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ABSTRACT

A new free interactive OpenGL software tool is demonstrated, that visualizes all monoclinic, and so far part of the orthorhombic, triclinic and hexagonal space group symmetries. The software computes with Clifford (geometric) algebra.
The space group visualizer originated as a script for the open source visual CLUCalc, which fully supports geometric algebra computation.
This paper briefly describes the historical and scientific developments leading to the space group visualizer project. Then we step by step demonstrate space group selection and the powerful set of interactive tools, including continuous free interactive 3D rotations, repositioning and resizing of the crystal domain in view. The most prominent feature of the space group visualizer is the full visualization of all spatial symmetries of a crystal domain. Beyond this the user can reduce the view to single symmetry operations or to certain classes of symmetries.

1. BACKGROUND

Geometry belongs to the seven ancient liberal arts practiced since Greek and Roman antiquity. The beauty of crystals on the other hand has equally long fascinated humans of all times. For Example the ancient Hebrew high priest had to wear 14 engraved precious stones (gems) to represent his nation before God. Geometry merges with the beauty of diamonds in the subject of crystallography, the study of the symmetry of regular crystals. Crystal symmetry reveals the abstract geometric beauty inside skillfully cut priceless jewels.
The so far prevailing mathematical formalism of crystal symmetry is tied to coordinates, vectors and matrices. These arrays of integers, fractions and variables hide the underlying mathematical beauty, like a thick cloak hides a brilliant gem necklace. In the middle of the 19th century mathematicians in Germany and Britain began to lift the cloak. They introduced the geometric product of vectors at the foundation of geometric algebra. At the end of the 20th century a Mexican student went on to write a thesis entitled: *Operaciones de simitria mediante algebra geometrica aplicadas a grupos cristalograficos* [1]. And finally at the beginning of the new millennium the American geometric algebra expert D. Hestenes lectured in Cambridge (UK) on *Point Groups and Space Groups in Geometric Algebra* [2]. This approach has been further expanded in [3].
At that time one of us had begun to develop CLUCalc, a visualization program for geometric algebra multivectors. Knowing of each other the idea formed to use CLUCalc in order to interactively illustrate the elegant principally coordinate free way how geometric algebra deals with point groups. In 2004 we therefore created a Point Group visualization script with CLUCalc [4], now freely available through the internet [5].
A year later we began using our experience with the symmetry of single crystal cells to develop interactive software for all known 230 symmetry groups of regular three-dimensional crystals, the *space group visualizer*. The mathematical engine of this program is geometric algebra, converted to high end computer graphics by CLUCalc. The result shows the geometric configuration of real crystals, the crystal lattice, the three vectors used by geometric algebra and all symmetries characterizing the crystal. Real physical beauty thus matches the fully developed abstract beauty of mathematics. The space group visualizer in a sense works like an accurate virtual microscope down to the atomic scale regarding the

constitution and symmetry of matter.

2. INTRODUCTION

In a number of previous publications we described both the geometric algebra background [4,6,7,8,9,10] and the use of the point group [4,11] and space group visualization scripts [8,12,13]. In the current paper we will build on these foundations and only focus on the visualization window of the space group visualizer. With descriptions of all window elements, all available tools and a range of sample figures we try to promote the use of the software.

3. USING THE SPACE GROUP VISUALIZER

3.1 The space group visualizer screen window

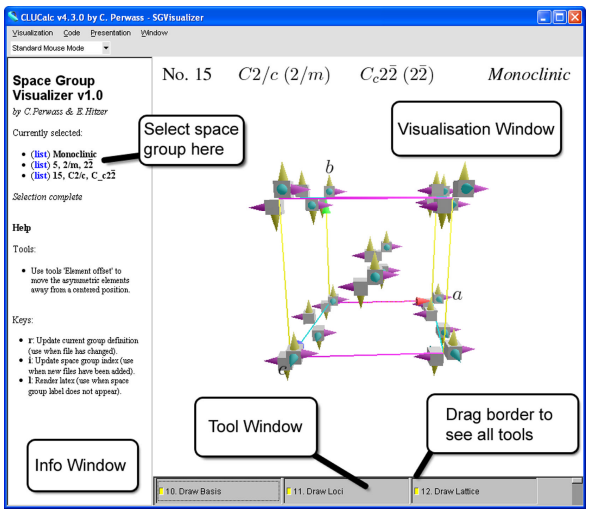

Fig. 1 Space Group Visualizer screen image.

The latest version of the space group visualizer (SGV) can be obtained from www.spacegroup.info. Clicking the download link downloads the executable installation file. Executing the installation file installs the space group visualizer in a dedicated program folder and deposits a shortcut to the space group visualizer software on the desktop of the computer. Clicking this desktop icon opens the visualization window (Fig. 1).
On the left this window has a vertical browser panel for selecting a specific space group. To the right we find the actual graphical visualization with a grey pull up tool sector at its bottom. Dragging up the upper border of the tool sector gives access to all available tools.

3.2 Choosing a symmetry group

The symmetry choice is done by first selecting one of the seven crystal systems (e.g. monoclinic, left side of Fig. 2) displayed in activated bold blue characters. The browser panel responds by displaying all point groups associated with the chosen crystal system (right side of Fig. 2). Table 1 contains a list of all 32 crystallographic point groups grouped according to the crystal type. The table lists the number of each point group (1-32), the geometric name symbol [2,3], the international name symbol (i.e. the abbreviated Hermann-Maugin symbol [14]), and the Schoenflies notation widely used in many textbooks.

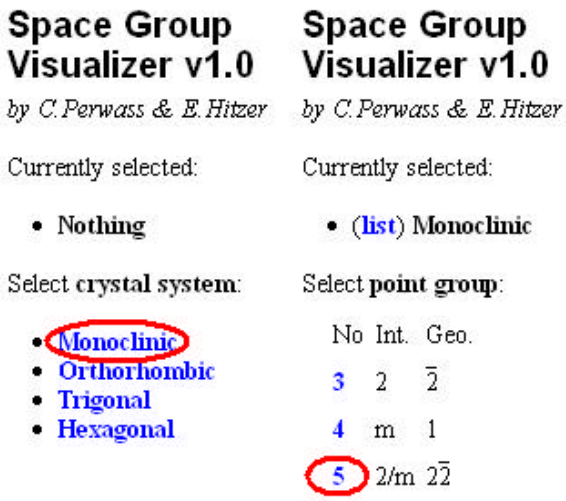

Fig. 2 Left side: Left SGV browser panel showing implemented **crystal systems**.
Right side: Selecting **Monoclinic** opens a list of monoclinic **point groups** [Number (No.), international (Int.) and geometric (Geo.) names.]

Now the user can chose the point group by clicking its bold blue number, as indicated in the right part of Fig. 2. This action will open a list of all space groups associated with the pre-chosen point group (see Fig. 3, left side). This interactive list (with numbers ranging from 1 to 230 for all space groups) lists the bold blue space group number, the geometric space group symbol [3] and the international space group symbol (abbreviated Hermann-Maugin notation, [14]).

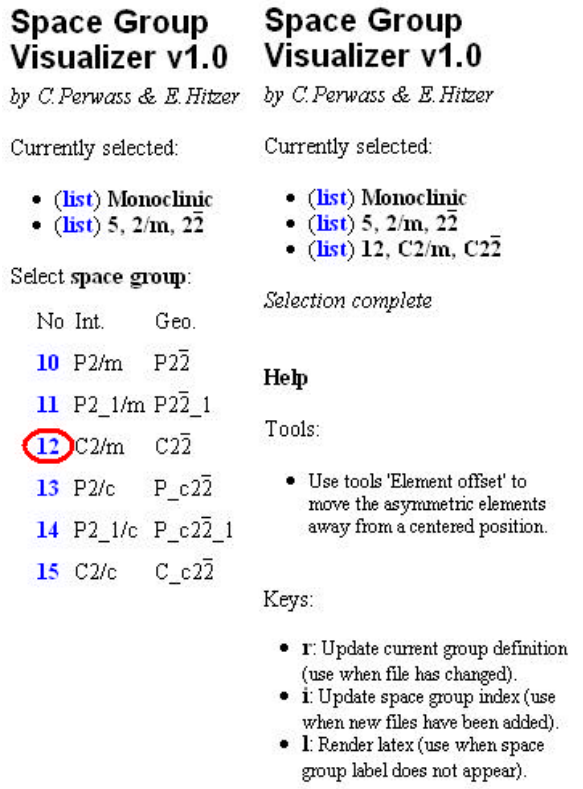

Fig. 3 Left side: After selecting a crystal system (here **Monoclinic**) specific point group all associated **space group**s appear [ITC number (No.), international (Int.) and geometric (Geo.) names]. Right side: Selection of a space group; showing the crystal system (here **Monoclinic**), the pre-selected point group (here No. **5**) and the finally selected space group (here No. **12**).

No. 12 $C2/m$ $(2/m)$ $C2\bar{2}$ $(2\bar{2})$ *Monoclinic*

Fig. 4 Space group information line at upper left corner of viewer window. Listing: Space group number, international name (with int. point group symbol in brackets), geometric name (with geom. point group symbol in brackets) and the crystal system.

Finally clicking on the bold blue space group number completes the space group selection as shown on the right side of Fig. 3. To the right of the browser panel appears simultaneously one full lattice cell with geometric vector basis, cell frame and a representative set of asymmetric general elements (grey cubes with three colored cones instead of atoms or molecules) in general locations (see e.g. Fig. 1).
The right of Fig. 3 shows three lines for the crystal system, the selected point group and the selected space group.

Table 1 Crystallographic point groups listed by crystal type, number (ordered as in [14]), international name, geometric name [2,3] and Schoenflies symbol.

Crystal type	ITC No.	Geom. Name	Int. Name	Schoen-flies
triclinic	1	$\bar{1}$	1	C_1
	2	$\overline{22}$	$\bar{1}$	C_i
mono-clinic	3	$\bar{2}$	2	C_2
	4	1	m	C_s
	5	$\bar{2}2$	$2/m$	C_{2h}
ortho-rhombic	6	$\bar{2}\bar{2}$	222	D_2
	7	2	$mm2$	C_{2v}
	8	22	mmm	D_{2h}
tetra-gonal	9	$\bar{4}$	4	C_4
	10	$\overline{42}$	$\bar{4}$	S_4
	11	$\bar{4}2$	$4/m$	C_{4h}
	12	$\bar{4}\bar{2}$	422	D_4
	13	4	$4mm$	C_{4v}
	14	$4\bar{2}$	$\bar{4}2m$	D_{2d}
	15	42	$4/mmm$	D_{4h}
trigonal	16	$\bar{3}$	3	C_3
	17	$\overline{62}$	$\bar{3}$	C_{3i}
	18	$\bar{3}\bar{2}$	32	D_3
	19	3	$3m$	C_{3v}
	20	$6\bar{2}$	$\bar{3}m$	D_{3d}
hexa-gonal	21	$\bar{6}$	6	C_6
	22	$\bar{3}2$	$\bar{6}$	C_{3h}
	23	$\bar{6}2$	$6/m$	C_{6h}
	24	$\bar{6}\bar{2}$	622	D_6
	25	6	$6mm$	C_{6v}
	26	32	$\bar{6}m2$	D_{3h}
	27	62	$6/mmm$	D_{6h}
cubic	28	$\bar{3}\bar{3}$	23	T
	29	$4\bar{3}$	$m\bar{3}$	T_h
	30	$\bar{4}\bar{3}$	432	O
	31	33	$\bar{4}3m$	T_d
	32	43	$m\bar{3}m$	O_h

Each line begins with the bold blue word “list”. Clicking on these lists brings the user back to one of the previous browser panels displaying the corresponding list. Below the message “selection complete” the user finds helpful hints on using tools and keys.

3.3 The space group information line

The visualization window to the right carries on its top the space group information line. An example for space group 12 is given in Fig. 4.
The space group number (between 1 and 230) is followed by the international space group name with the international point group symbol in brackets. Next follows the geometric space group name with the geometric point group symbol in brackets and finally the name of the crystal system to which the space group belongs.

3.4 The visualized crystal domain graphics

The spatial crystal domain in the center of the visualization (see e.g. Fig. 1) shows the three generating vectors (a,b,c in blue, green and red, respectively). It further shows a (lattice) wire frame (purple and yellow) for one complete cell and it finally shows a representative set of general elements (grey cube with three colored cones) in general positions. The symmetry of these positions is represented by the chosen symmetry (space) group. With the mouse buttons and the shift key one can freely rotate, translate and scale the visualization in 3D. The tools of the bottom tool window allow the user to further manipulate the visualized crystal domain, including the full visualization of all symmetry elements located in the displayed crystal domain.

Fig. 5 Tools for drawing the geometric vector basis, general positions (loci), and one cell lattice (wire) frame.

3.5 The general tool box

The tool window at the bottom can be dragged up to gain access to all available tools. The full tool box contains a number of tools that allow to modify the visualization: Draw Basis, Loci (general postions), and Lattice; Lattice Type, selected Generators, Symmetry Generator (operations), Symmetry Elements (by Type), 3D Cell Count, Color and Lighting, 3D Element Offset, cell Angles, and side Lengths.

3.5.1 Basis, loci and lattice

The lattice basis, the points in general positions and the cell lattice can be clicked on and off (comp. Fig. 5).
Fig. 6 has a lattice (wire frame) for the cell pictured. There the Draw Lattice function tool is switched on. In Fig. 7 no lattice appears, the Draw Lattice tool is switched off.

3.5.2 Cell count, element offset

The user has the freedom to change the extension of the lattice domain in every direction.

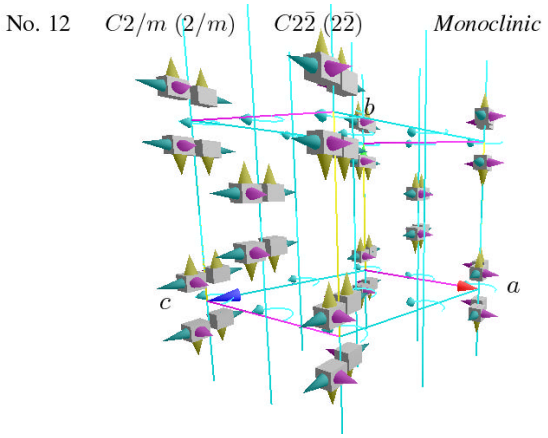

Fig. 6 Rotations (axis and angles).

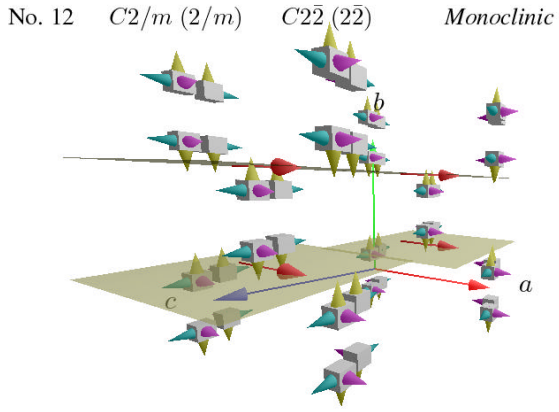

Fig. 7 Glide reflections (reflection plane and half translation in plane).

The sliders which allow to increase the number of visualized cells in three directions (X, Y and Z) are shown in Fig. 8. They have a range between 0 and 5, numerically indicated on the left side of each slider. Figures 9, 10 and 11

show maximum extended cells in one, two and three directions respectively.

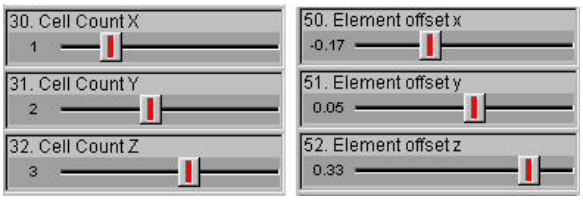

Fig. 8 Cell count (X,Y,Z) and offset (x,y,z) tools.

No. 144 $P3_1$ (3) $P\bar{3}_1$ ($\bar{3}$) *Trigonal*

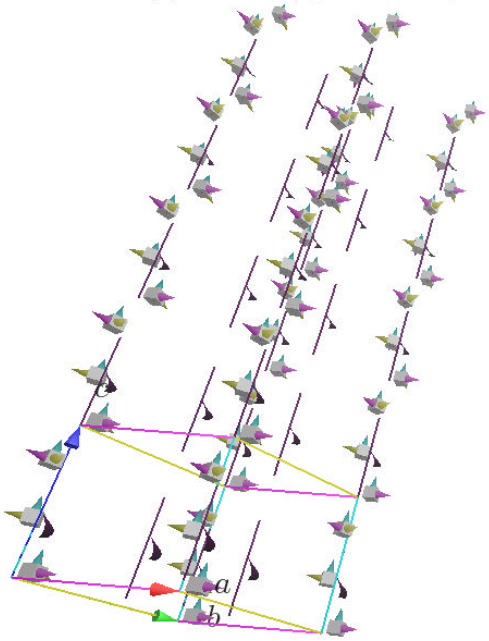

Fig. 9 Five cell one dimensional extension of trigonal crystal with three fold screw axis.

Figure 8 (right side) also shows the three sliders in order to offset the position of the representative general elements (grey cubes with colored cones). This allows e.g. to graphically demonstrate Wyckoff positions (i.e. locations of higher symmetry). Or it can be used to understand how symmetry related general positions (e.g. related by a reflection) vary with the position of a general element.

3.5.3 Changing cell parameters: lengths and angles

Depending on the crystal system all, some or none of the three cell angles are unrestricted. For example in the monoclinic case two angles are restricted to 90 degrees, the third angle is free. If free angles exist, they can be varied with sliders as in the top of Fig. 12, the numerical values (in degrees) are again indicated on the left side of each slider.

No. 168 $P6$ (6) $P\bar{6}$ ($\bar{6}$) *Hexagonal*

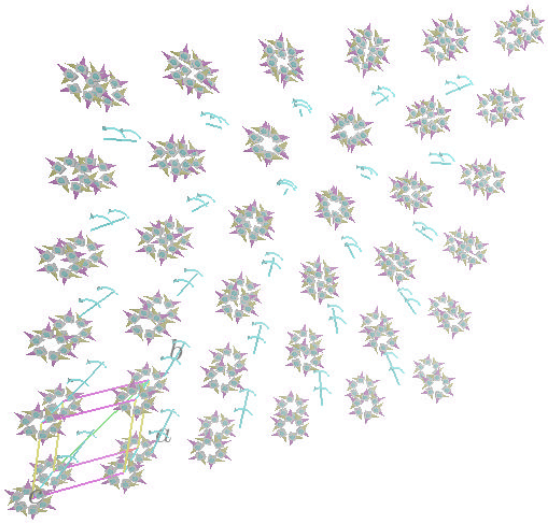

Fig. 10 Five by five cell two dimensional extension of hexagonal crystal domain. A resulting threefold rotation axis is also shown.

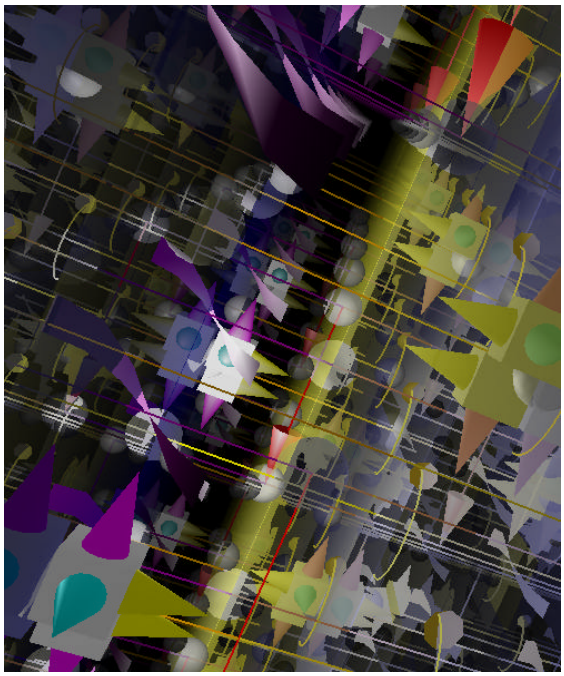

Fig. 11 Inside a five by five by five cell domain of a monoclinic crystal. All symmetries are shown, black background and central lighting are used.

One cell edge length is always free. In some cases it may be two or even all three. The free

edge lengths can be varied with sliders named Len a, Len b, and Len c as shown in Fig. 12. The numerical edge lengths are indicated in relative length units on the left side of each slider.

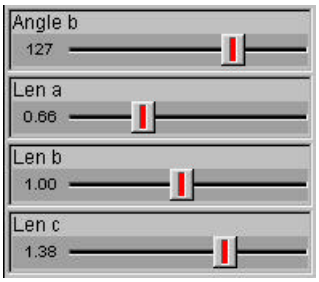

Fig. 12 Sliders for changing free cell angles (here e.g. angle b), and lengths of cell edges.

3.5.4 Background color and ligthting

Depending on the purpose of the use of the space group visualizer it may be better to have a black background (for interactive use, for presentations, etc.) or a white background for producing figures for publications, etc. The background color scheme achieves this. Its tool menu is shown in Fig. 13. Change of scheme is done be clicking on the current scheme. A two line context menu opens, offering the two implemented schemes.

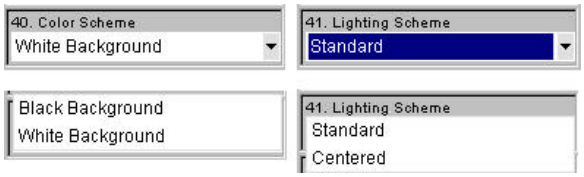

Fig. 13 Background color schemes (left) and lighting schemes (right). Clicking on the menu bars produces two line context menus for scheme selection.

The standard for lighting is to have constant luminosity throughout the crystal domain pictures in the visualizer. Yet in the case of cells with symmetry planes or for larger domains the user may loose orientation due to the many visual elements in view. For such situations the centered light scheme highlights a central spherical domain with radially decreasing luminosity. Clicking on the status line in the lighting scheme menu opens the two line context menu for changing the scheme (comp. right side of Fig. 13). All figures in this paper use the standard lighting scheme, except Fig. 11 which has centered lighting.

3.5.5 Lattice type

This tool has the purpose of allowing the user to view the same crystal with different ways of assigning lattice cells. Historically and practically a variety of lattice choices are in use [14]. The geometric algebra approach also has some implications for positioning lattices, e.g. by offsetting the origin of the lattice by a constant fractional combination of elementary lattice translations, etc. Fig. 14 shows the lattice choice in the top left menu item. In the future the lattice type will provide further non-standard lattice choices.

3.6 Symmetry generator tools

Now we treat the most interesting and distinguished features of the space group visualizer: Its ability to select and display each single symmetry present in a crystal cell (or domain) one by one, in groups, or a total combination of all symmetries.

3.6.1 Basis generator menu

Each symmetry operation in a space group is an elementary combination of reflections and translations. A pair of reflections typically forms a rotation, a triple of reflections a rotary reflection, etc. Great mathematical beauty is revealed in the fact that for each space group a very limited set of a handful of generators suffices to generate the whole infinite space group.
This generator basis set always includes the identity and three elementary translations *Ta*, *Tb*, and *Tc*.
The selected generators form a generator basis of the space group. Their choice and visualization is one by one. Beyond this space groups may contain point symmetry elements: namely reflections (indicated by vectors normal to the mirror plane), rotations (indicated by a pair of vectors in the plane of rotation), rotary reflections (indicated by a vector triple). All these have in common, that they leave at least one point invariant. Special combinations of these point symmetries with fractional translations lead to glide reflections (a reflection followed by a half translation in the plane of reflection) and screw displacements (a rotation followed by a fractional translation in the

direction of the rotation axis).
The default view of the crystal cell shows no (none) symmetry generator. Clicking on the word “None” in the (basis) Generator menu line opens a pop-up context menu with a complete list of all basic generators necessary to generate the selected space group. Selection of any of these generators visualizes the generator immediately in the crystal cell. For example selection of a normal vector will immediately display the plane of reflection, etc.
This function corresponds to the entries in “Generators selected” in [14], though geometric algebra may naturally lead to a different choice of basic generators [3].

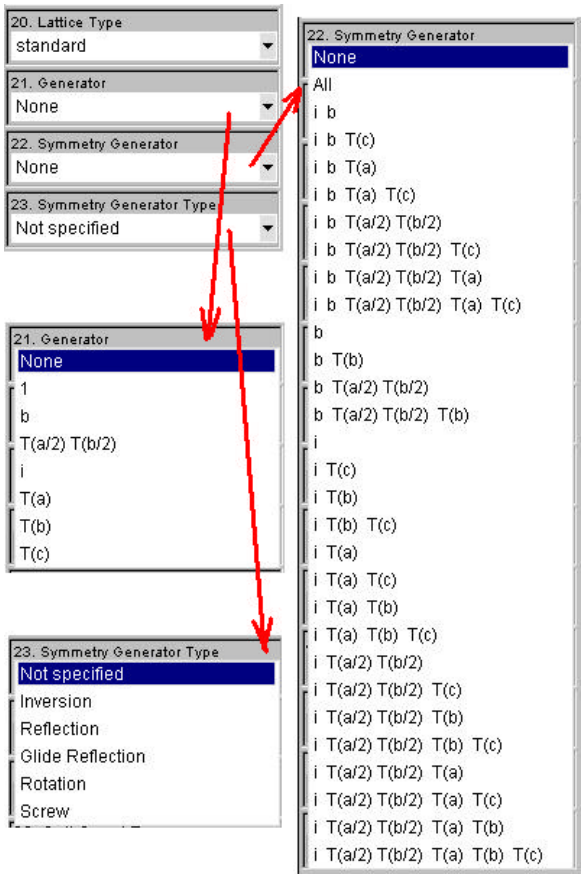

Fig. 14 Lattice type, (space group basis) generator tool, (full space group) symmetry generator (symmetry elements) tool and symmetry type selection tool. The red arrows indicate context menus activated by clicking on the one line tools.

3.6.2 All symmetry elements of a crystal cell domain – one by one

The product of two symmetry elements typically leads to a new symmetry element. For example the product of a reflection with a translation leads either to a new shifted reflection plane or to a glide reflection, etc. Each space group has its own characteristic set of symmetries within each cell. Positioning one general element (indicated as a grey cube with colored cones) in a crystal cell permits to generate all other general elements in the cell by applying the symmetry operations characteristic for each cell. So either the characteristic spatial arrangements of the general elements (default view, e.g. Fig. 1) characterizes a crystal and its space group or the set of all symmetries present in the cell.
The space group visualizer allows the user both approaches. The spatial arrangement of general elements is the default (e.g. Fig. 1). By choosing “All” instead of “None” from the symmetry generator context menu (right side of Fig. 14), the user can add all symmetry elements of the crystal domain in view. Clicking the Draw Loci tool of Fig. 5 makes it possible to delete/show the general elements (the spatial lattice represented by grey cubes with colored cones). Without the general elements the user gets a pure view of all symmetries present.
The list of symmetries located in a single crystal cell can already be very long. The symmetry generator context menu allows to one by one select each and every symmetry element and interactively view its graphical depiction in three dimensions in the actual crystal cell view. This function goes far beyond the traditional table and diagram form of the International Tables of Crystallography [14].

3.6.3 Crystal symmetry elements display by type

The variety and richness of symmetry of even a single crystal cell domain can be bewildering. For bringing order into the zoo of symmetries the space group visualizer offers symmetry (generator) element display by five types: Inversion, Reflection, Glide Reflection, Rotation and Screw types are available. The default is “Not specified”, i.e. no symmetries are excluded by default. Choosing the type inversion will restrict the display of symmetries to inversions as in Fig. 15. The actual display shows a small grey ball centered at each center of inversion.
Choosing the type glide reflection will restrict the display of symmetries to glide reflections as in Fig. 7. Glide reflections show the colored semi-transparent plane of reflection and the half

translation vector in the plane of reflection.
Choosing the type rotation will restrict the display of symmetries to rotations as in Fig. 6. A rotation is indicated by the rotation axis and a directed arc indicating the angle of the rotation. Depending on the color scheme, the arcs are also color coded (characteristic colors for 30, 60, 90, and 120 degrees).

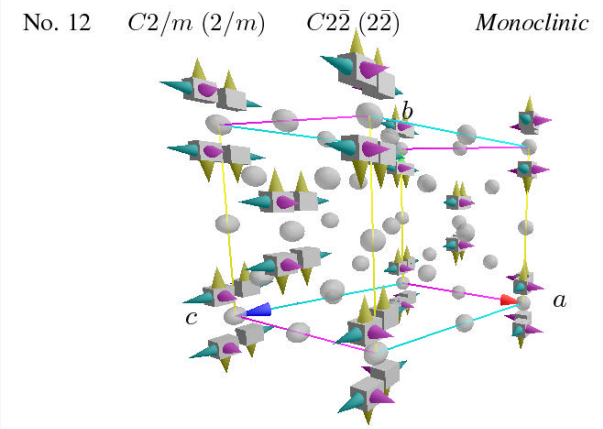

Fig. 15 Centers of inversion.

Choosing the type reflection will restrict the display of symmetries to reflections as in Fig. 16. The reflection planes (mirrors) are shown as semi-transparent planes.

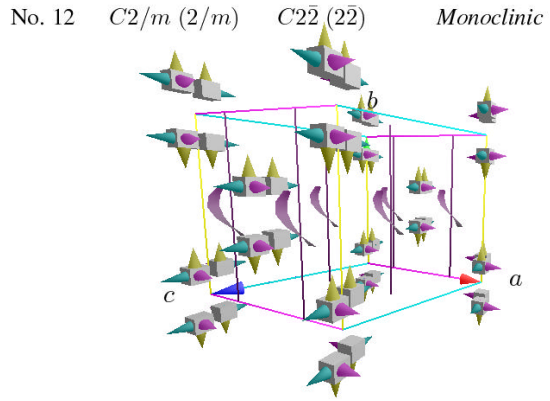

Fig. 16 Planes of reflection. In this monoclinic example the planes are all normal to vector b.

Finally choosing the type screw (=screw rotation) will restrict the display of symmetries to screws (also called twists) as in Figures 9 and 17. A screw is indicated by the screw rotation axis and an small spiral winding into the direction of the axial displacement around the axis of the screw. Viewing a screw in direction of its axis shows that the spiral covers exactly the angle of the rotation associated with the screw.

3.7 Three dimensional interactivity

The advanced interactive OpenGL computer graphics features allow the user to use the right and left mouse buttons in combination with the shift key for continuous free interactive 3D rotations, repositioning and scaling of the crystal domain in view. This provides a second important feature going far beyond the traditional table and diagram approach of [14].

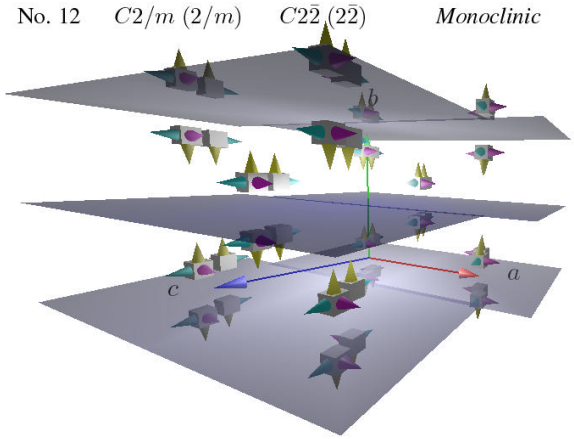

Fig. 17 Screw rotations (rotation axis, angles, and axial translation).

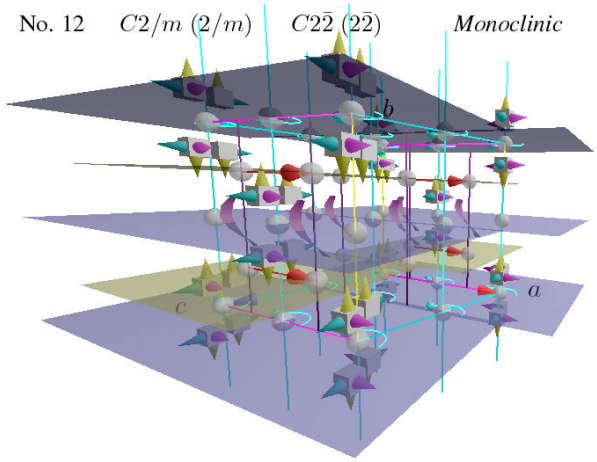

Fig. 18 Combined view of cell with all general elements and all symmetries.

3.8 All in one

Finally Figs. 11 and 18 show the total combination of all general elements and all symmetry elements of a crystal cell domain or a

single crystal cell. Fig. 11 shows an extended crystal region with black background and central lighting. Whereas Fig. 18 concentrates on a single crystal cell with white background and standard light scheme. Fig. 11 is the typical interactive view and Fig. 18 represents a view which may be more suitable for publications.

4. FUTURE

We have formed a small active and dedicated international development team with the aim of completing the space group visualizer for all 230 space groups. Our aim is to comply as fully as possible with the needs of crystallographers around the globe. We want to optimize the usefulness of the space group visualizer for all practical purposes, including research, demonstrations, study and teaching. For us it is the most promising candidate to increase and spread the knowledge and appreciation of the beauty of crystals, regarding their physical beauty as well as the abstract beauty of the enormous degree of symmetry involved.
Future options will possibly be custom made general elements (e.g. balls and linkage groups graphically representing atoms, ions and molecules [anorganic and organic]). Further work needs to be done on the implementation of non-standard lattices. Suggestions of new desired features are highly welcome and will be duly considered.

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