Interactive Visualization of Plane Space Groups with the Space Group Visualizer

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1 Introduction

This set of instructions shows how to successfully display the 17 two-dimensional (2D) space groups in the interactive crystal symmetry software Space Group Visualizer (SGV) [6]. The SGV is described in [4]. It is based on a new type of powerful geometric algebra visualization platform [5].

The principle is to select in the SGV a three-dimensional super space group and by orthogonal projection produce a view of the desired plane 2D space group. The choice of 3D super space group is summarized in the lookup table Table 1. The direction of view for the orthographic projection needs to be adapted only for displaying the plane 2D space groups Nos. 3, 4 and 5. In all other cases space group selection followed by orthographic projection immediately displays one cell of the desired plane 2D space group.

The full symmetry selection, interactivity and animation features for 3D space groups offered by the SGV software become thus also available for plane 2D space groups. A special advantage of this visualization method is, that by canceling the orthographic projection (remove the tick mark of Orthographic View in drop down menu Visualization), every plane 2D space group is seen to be a *subgroup* of a corresponding 3D super space group.

The convenient lookup table Table 1 lists column by column: 2D crystal system, the 2D space group number [1], the Hermann-Maugin name of the 2D space group [1], (and the Coxeter-Hestenes-Holt symbols [2, 3] in brackets) the crystal system of 3D super space group, the 3D point group number of the 3D super space group [1], the 3D space super group number [1], and the the Hermann-Maugin name of the 3D space super group (and the Coxeter-Hestenes-Holt symbols [2, 3] in brackets).

The colors become much more vivid with a choice of a black background, which is strongly recommended for presentations: Drop down menu Visualization, Color Scheme, Black Background. For printability this set of instructions uses white background pictures created with the SGV.

The SGV can be purchased from [7]. The current instructions apply to the Space Group Visualizer, version 2.2.5.

2 The 17 plane space groups

2.1 Oblique plane space groups

2.1.1 No. 1: $p1$ $(p\bar{1})$

What to do?

- Open the **SGV**.
- **Select** from the left selection panel: Triclinic, point group 1, space group 1. Compare line 1 of lookup table Table 1.
- In the toolbar adjust the first **two angles to** 90°.

Table 1: *Lookup table for the 17 2D space groups.* Column 1: 2D crystal system. Column 2: 2D space group number. [1] Column 3: Hermann-Maugin name of 2D space group [1], and Coxeter-Hestenes-Holt symbols [2, 3] in brackets. Column 4: Crystal system of 3D super space group. Column 5: 3D point group number of 3D super space group. [1] Column 6: 3D space super group number. [1] Column 7: Hermann-Maugin name of 3D space super group and Coxeter-Hestenes-Holt symbols [2, 3] in brackets. This 3D super space group needs to be selected in the SGV in order to display the 2D space group by orthographic projection.

2D plane space groups			**3D space super groups**			
2D cry. sys.	2D#	2D SG name	3D cry. sys.	3D PG#	3D SG#	3D SG name
Oblique	1	$p1$ $(p\bar{1})$	Triclinic	1	1	$P1$ $(P\bar{1})$
(anorthic)	2	$p2$ $(p\bar{2})$	Monoclinic	3	3	$P2$ $(P\bar{1})$
	3	pm $(p1)$	Monoclinic	4	6	Pm $(P1)$
	4	pg (p_g1)	Monoclinic	4	7	Pc (P_c1)
	5	cm $(c1)$	Monoclinic	4	8	Cm $(C1)$
Rectangular	6	$p2mm$ $(p2)$	Orthorhombic	7	25	$Pmm2$ $(P2)$
	7	$p2mg$ (p_g2)	Orthorhombic	7	28	$Pma2$ $(P2_a)$
	8	$p2gg$ (p_g2_g)	Orthorhombic	7	32	$Pba2$ (P_b2_a)
	9	$c2mm$ $(c2)$	Orthorhombic	7	35	$Cmm2$ $(C2)$
	10	$p4$ $(p\bar{4})$	Tetragonal	9	75	$P4$ $(P\bar{4})$
Square	11	$p4mm$ $(p4)$	Tetragonal	13	99	$P4mm$ $(P4)$
	12	$p4g$ (p_g4)	Tetragonal	13	100	$P4bm$ (P_b4)
	13	$p3$ $(p\bar{3})$	Trigonal	16	143	$P3$ $(P\bar{3})$
Hexagonal	14	$p3m1$ $(p3)$	Trigonal	19	156	$P3m1$ $(P3)$
	15	$p31m$ $(h3)$	Trigonal	19	157	$P31m$ $(H3)$
	16	$p6$ $(p\bar{6})$	Hexagonal	21	168	$P6$ $(P\bar{6})$
	17	$p6m$ $(p6)$	Hexagonal	25	183	$P6mm$ $(P6)$

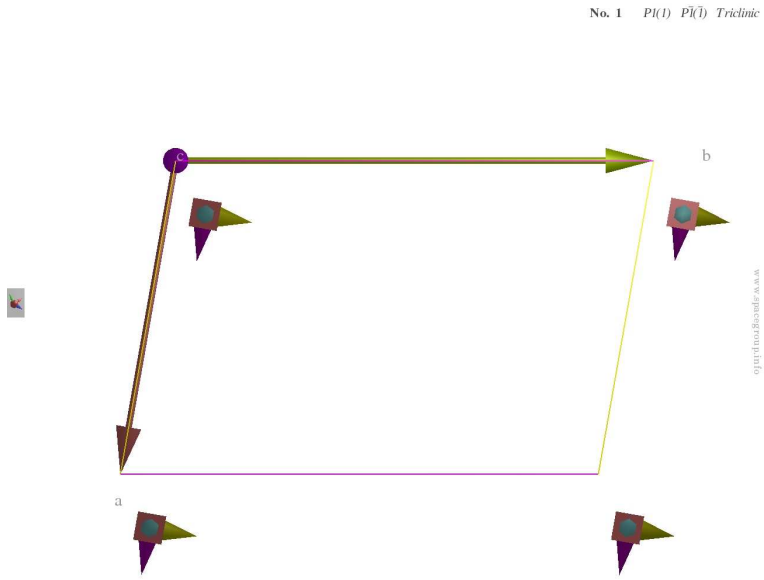

Figure 1: SGV view of 2D oblique space group $p1$ ($p\bar{1}$).

- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p1$ appears, see Fig. 1.

Tips for what else to do.

- Clicking on the **general element symbol** (gray cube with colored cones) in the toolbar removes/shows the general elements.
- The **size of the general elements** can be reduced from the initial 100%.
- The 2D **cell/lattice frame** can be toggled on/off.
- The **number of cells** in the a and b directions can be changed between 0 and 5, see Fig. 2 shows 3×3 cells.
- In order to keep the cells in view press Ctrl+right mouse button to **scale the scene**. For better **visibility** the SGV may blend out some visualization elements. This can be adjusted by moving the mouse, while pressing the right mouse button (without the Ctrl key!).
- Alternatively the **axis length** a and b can be changed.
- The visualization of the **generating vectors** a and b can be switched on/off.

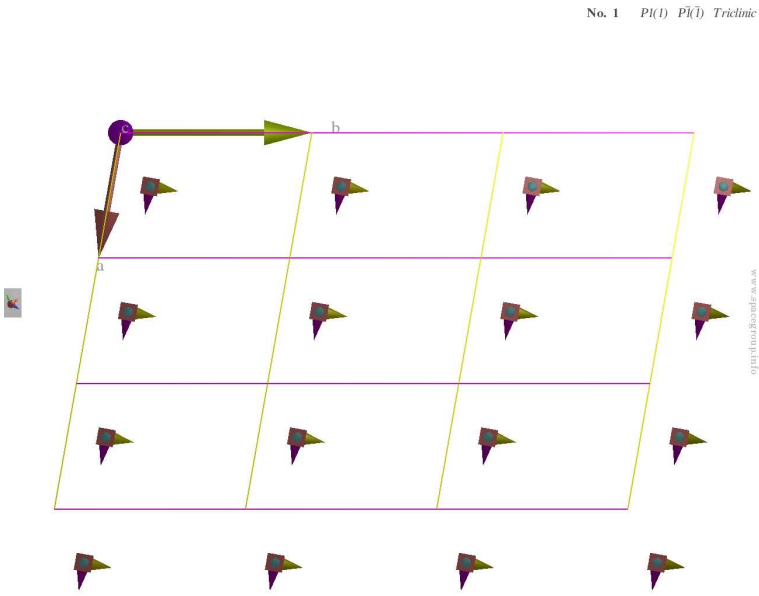

Figure 2: SGV view of 3×3 cells of 2D oblique space group $p1$ ($p\bar{1}$).

- The **cell angle** (3rd angle in the toolbar list) can be modified.
- With Shift+right mouse button held down, the **whole view can be moved** up/down and left/right with the mouse.
- With first placing the mouse pointer over a general element and then Shift+right mouse button held down, the **general element can be moved** up/down and left/right with the mouse. Translation symmetry is observed.
- With drop down menu Visualization, Reset Loci Position (or Ctrl+l), the **general elements** can be set back to their **default positions** and orientation.
- Still **images can be saved**: Select either Save View (possible formats: PNG, PNG with bounding box, JPEG, Bitmap, Postscript, JPEG+EPS combined) or Quick Save View in the drop down menu File.
- The **visualization context help** at the bottom of the visualization window can be switched off/on with Ctrl+h.

2.1.2 No. 2: $p2$ ($p\bar{2}$)

What to do?

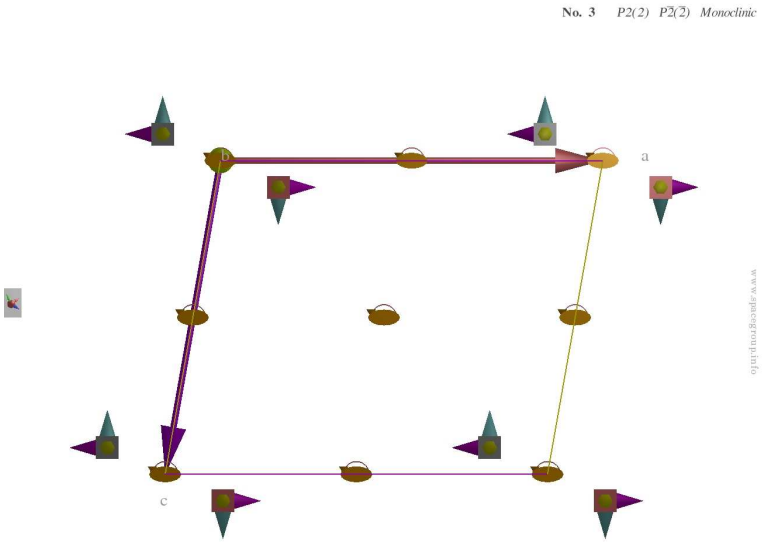

Figure 3: SGV view of 2D oblique space group $p2$ $(p\bar{2})$.

- **Select** from the left selection panel: Monoclinic, point group 3, space group 3. Compare line 2 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.
- Suggestion: **adjust length** of horizontal axis a.

Now one 2D cell of $p2$ appears, see Fig. 3. Fig. 4 shows 3×3 cells.

Tips for what else to do.

- By moving the mouse pointer over a rotation center symmetry symbol, the rotation is **animated**. This feature can be switched off (apart from the rotation of the symbol itself) by deselecting in drop down menu Visualization the box Animate Loci Symmetry.
- In the left panel selection menu, the **rotation symbols can now be selected** by location (in fractional coordinates) and by generator. The rotation generator is denoted by its geometric algebra representation (not by a 4×4 matrix), but can be easily identified from its data of Angle (A), Orientation (O), and Location (L).
- By left clicking on one rotation symbol all other **symbols** are **deselected**.
- By right clicking on one rotation **symbol** it **disappears**.

Figure 4: SGV view of 3×3 cells of 2D oblique space group $p2$ $(p\bar{2})$.

- Clicking all next to Location or Generator in the menu **brings back all rotation symbols**. The same happens when placing the mouse pointer over a remaining rotation symmetry symbol and pressing Ctrl+left mouse button.
- Compare also Section 2.1.1 on what else to do.

2.2 Rectangular plane space groups

2.2.1 No. 3: *pm* $(p1)$

What to do?

- **Select** from the left selection panel: Monoclinic, point group 4, space group 6. Compare line 3 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.
- Use right mouse button pressed (or Shift+right mouse button pressed for alternative direction) to **rotate the view**, such that vectors c (or a) points in or out of the screen.
- Optionally the **remaining angle** ($\neq 90°$) can be set to $90°$.

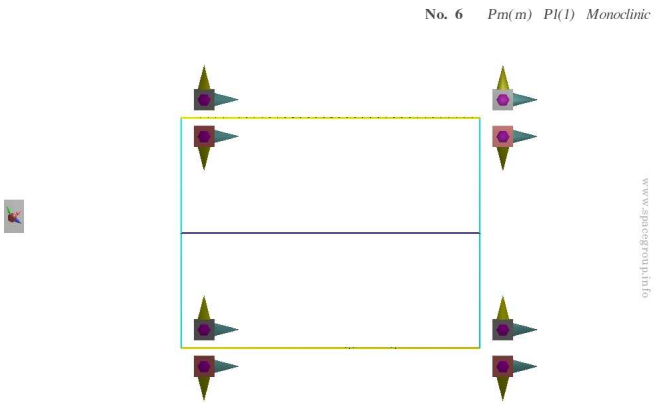

Figure 5: SGV view of 2D rectangular space group *pm* $(p1)$.

Now one 2D cell of *pm* appears, see Fig. 5. Fig. 6 shows 3×3 cells.

Tips for what else to do.

- The reflections can be **animated** similar to the rotations in section 2.1.2.
- The **reflections** can also be **(de)selected** similar to the rotations in section 2.1.2.

2.2.2 No. 4: *pg* (p_g1)

What to do?

- **Select** from the left selection panel: Monoclinic, point group 4, space group 7. Compare line 4 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.
- Use right mouse button pressed (or Shift+right mouse button pressed for alternative direction) to **rotate the view**, such that vectors a points in or out of the screen.

Now one 2D cell of *pg* appears, see Fig. 7. Fig. 8 shows 3×3 cells. The glide vectors appear symbolically in red along the yellow glide lines.

Tips for what else to do.

- The **glide reflections** can be **animated** similar to the rotations in section 2.1.2.
- The **glide reflections** can also be **(de)selected** similar to the rotations in section 2.1.2.

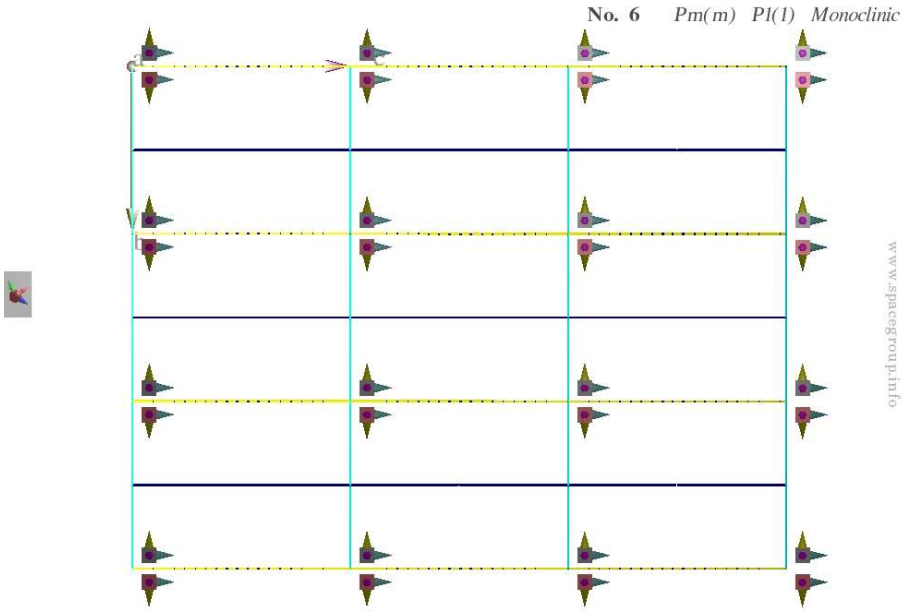

Figure 6: SGV view of 3×3 cells of 2D rectangular space group *pm* $(p1)$.

2.2.3 No. 5: *cm* $(c1)$

What to do?

- **Select** from the left selection panel: Monoclinic, point group 4, space group 8. Compare line 5 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.
- Use right mouse button pressed (or Shift+right mouse button pressed for alternative direction) to **rotate the view**, such that vectors c points in or out of the screen.
- Optionally adjust the **length of axis** a.
- Optionally the **remaining angle** ($\neq 90°$) can be set to $90°$.

Now one 2D cell of *cm* appears, see Fig. 9. Fig. 10 shows 3×3 cells. Reflection lines: blue, glide lines: yellow with red glide vectors.

Tips for what else to do.

- All **symmetry elements can be shown/removed** by selecting all/none in the line next to Symmetries in the left selection panel.

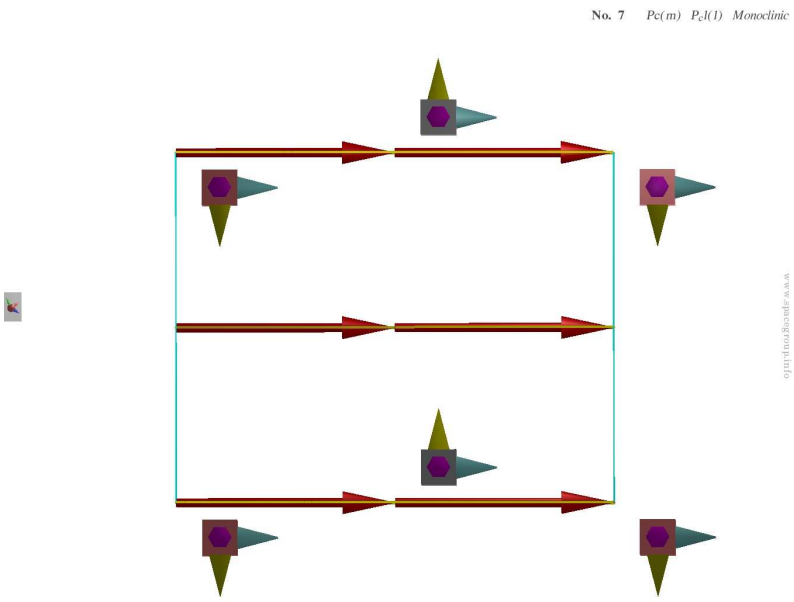

Figure 7: SGV view of 2D rectangular space group pg (p_g1).

- Now both types of **symmetry elements** (reflections and glide reflections) can be **selected and animated** directly with mouse interaction.
- Try the **options** only, other, all, none, select next to the items Reflection and Glide Reflection in the selection panel on the left.
- If the option select is chosen in both cases any combination of **reflections and glide reflections can be subselected** for display.

2.2.4 No. 6: $p2mm$ $(p2)$

What to do?

- **Select** from the left selection panel: Orthorhombic, point group 7, space group 25. Compare line 6 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p2mm$ appears, see Fig. 11. Fig. 12 shows 3×3 cells. Rotation centers and lines of reflection symmetry (blue) can be clearly seen.

Tips for what else to do.

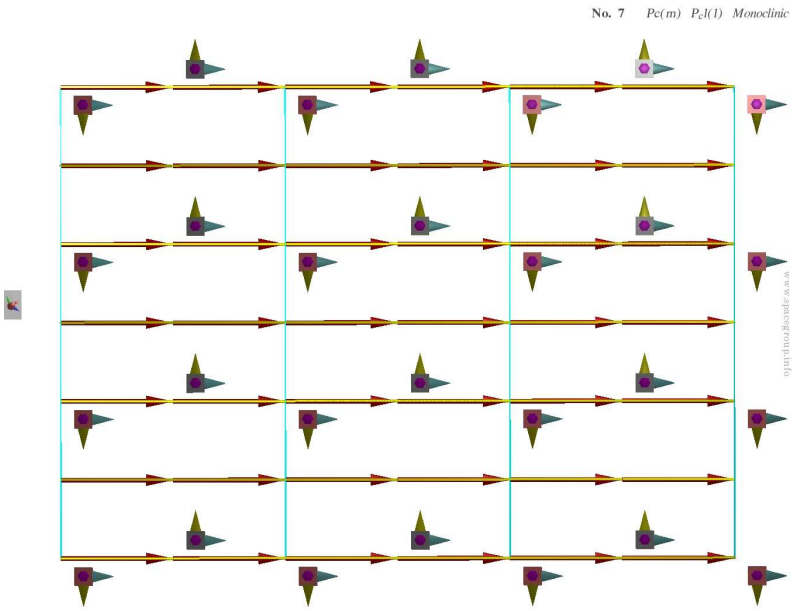

Figure 8: SGV view of 3×3 cells of 2D rectangular space group pg (p_g1).

- Now both types of **symmetry elements** (reflections and rotations) can be **selected and animated** directly with mouse interaction.
- Try the **options** only, other, all, none, select next to the items Reflection and Rotation in the selection panel on the left.
- If the option select is chosen in both cases any combination of **reflections and rotations can be subselected** for display.
- Deselecting the optional **cell/lattice frame** gives a clearer view of the lines of reflection symmetry.
- The **generating vectors** a and b which span the cell can easily be shown/removed by clicking on the vector icon in the toolbar.

2.2.5 No. 7: $p2mg$ (p_g2)

What to do?

- **Select** from the left selection panel: Orthorhombic, point group 7, space group 28. Compare line 7 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

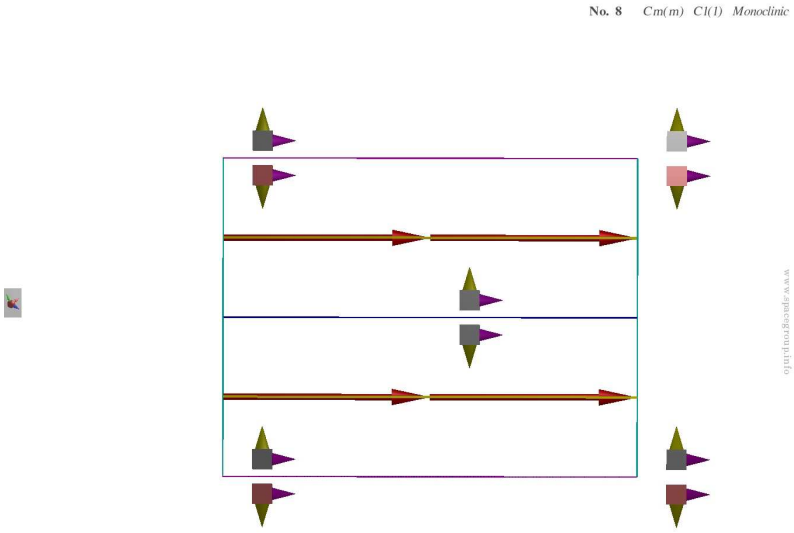

Figure 9: SGV view of 2D rectangular space group *cm* $(c1)$.

Now one 2D cell of *p2mg* appears, see Fig. 13. Fig. 14 shows 3×3 cells. Rotation centers, lines of reflection symmetry (blue), and lines of glide reflection (yellow) with red glide vectors can be clearly seen.

2.2.6 No. 8: *p2gg* $(p_g 2_g)$

What to do?

- **Select** from the left selection panel: Orthorhombic, point group 7, space group 32. Compare line 8 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of *p2gg* appears, see Fig. 15. Fig. 16 shows 2×2 cells. Rotation centers, and lines of glide reflection (yellow) with red glide vectors can be clearly seen.

2.2.7 No. 9: *c2mm* $(c2)$

What to do?

- **Select** from the left selection panel: Orthorhombic, point group 7, space group 32. Compare line 9 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

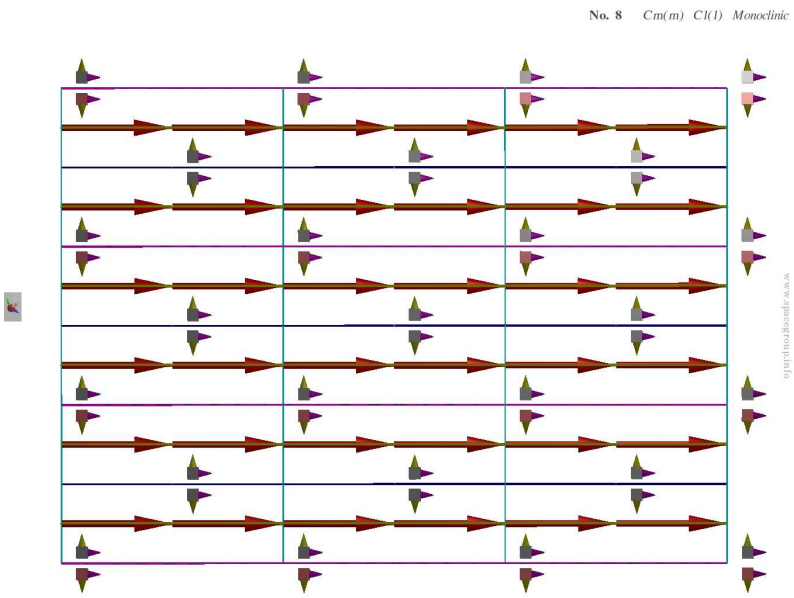

Figure 10: SGV view of 3×3 cells of 2D rectangular space group *cm* $(c1)$.

Now one 2D cell of *c*2*mm* appears, see Fig. 17. Fig. 18 shows 2×2 cells. Rotation centers, reflection lines (blue), and lines of glide reflection (yellow) with red glide vectors can be clearly seen.

Tips for what else to do.

- Deselecting the optional **cell/lattice frame** gives a clearer view of the lines of reflection symmetry.
- The **vectors** *a* and *b* which span the cell can easily be shown/removed by clicking on the vector icon in the toolbar.

2.3 Square plane space groups

2.3.1 No. 10: $p4$ $(p\bar{4})$

What to do?

- **Select** from the left selection panel: Tetragonal, point group 9, space group 75. Compare line 10 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

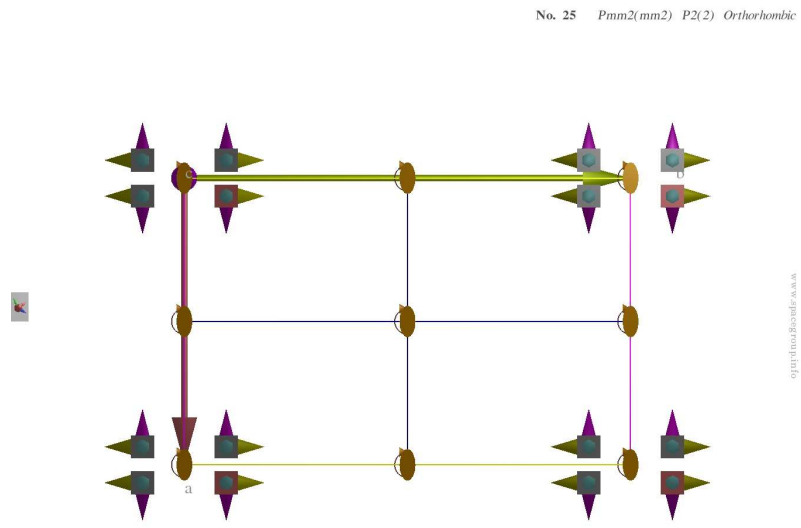

Figure 11: SGV view of 2D rectangular space group $p2mm$ $(p2)$.

Now one 2D cell of $p4$ appears, see Fig. 19. Fig. 20 shows 2 cells. Symbols for rotation centers appear color coded for 90° (small violet squares) and 180° (small brown ellipses) together with arc segments indicating the angle of rotation.

Tips for what else to do.

- Rotations can now additionally be **subselected by angle** in the left selection panel. Successively click Symmetries[select], Rotation[select], Angle[select].

2.3.2 No. 11: $p4mm$ $(p4)$

What to do?

- **Select** from the left selection panel: Tetragonal, point group 13, space group 99. Compare line 11 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p4mm$ appears, see Fig. 21. Fig. 22 shows two cells. Symbols for lines of reflection (blue), lines of glide reflection (yellow) with red translation component arrows, and for rotation centers (shape and color coded) appear.

Tips for what else to do.

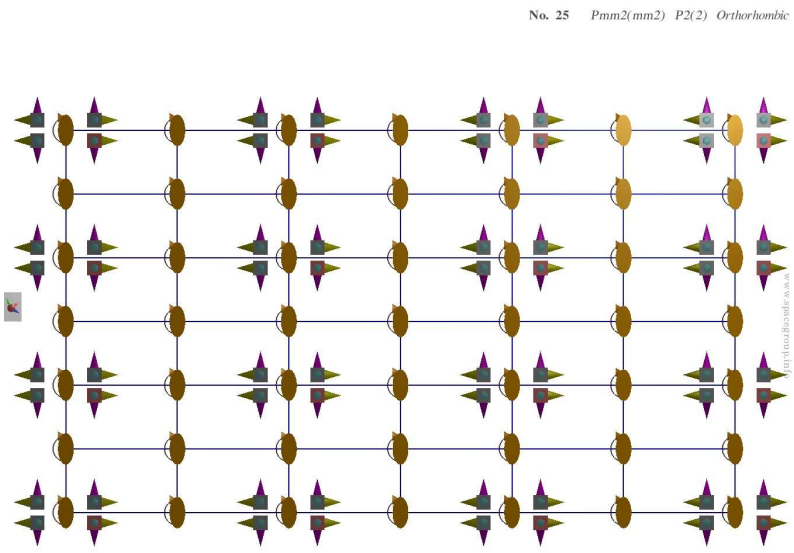

Figure 12: SGV view of 3×3 cells of 2D rectangular space group $p2mm$ $(p2)$.

- Reflection lines and glide reflection lines can be **subselected** according to **orientation** of their normal vectors, **location**, and **generator** expression.
- Additionally, the lines of glide reflection can be **subselected** by their **translation component**.
- Switching off the **cell/lattice frame** shows the horizontal and vertical lines of reflection clearly.
- Clicking the **general element icon** in the toolbar removes/shows the general element symbols (colored cube-cones).

2.3.3 No. 12: $p4gm$ (p_g4)

What to do?

- **Select** from the left selection panel: Tetragonal, point group 13, space group 100. Compare line 12 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p4gm$ appears, see Fig. 23. Fig. 24 shows two cells. Symbols for lines of reflection (blue), lines of glide reflection (yellow) with red translation component arrows, and for rotation centers (shape and color coded) appear.

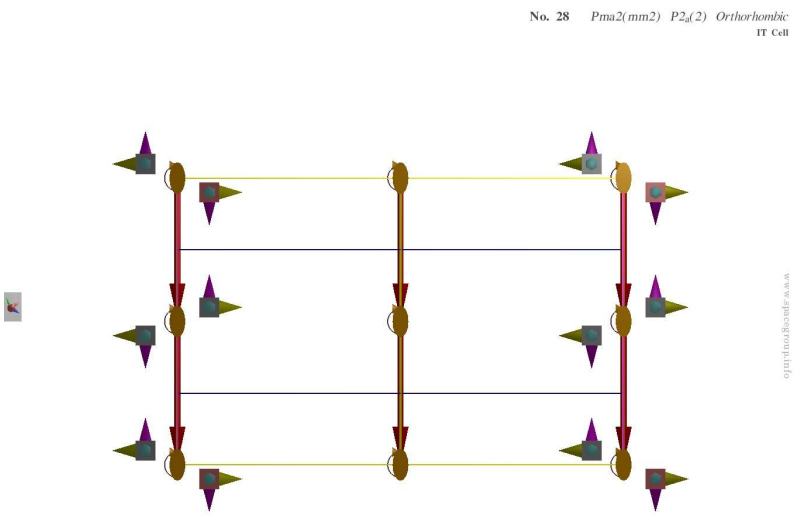

Figure 13: SGV view of 2D rectangular space group $p2mg$ (p_g2).

2.4 Hexagonal plane space groups

2.4.1 No. 13: $p3$ $(p\bar{3})$

What to do?

- **Select** from the left selection panel: Trigonal, point group 16, space group 143. Compare line 13 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p3$ appears, see Fig. 25. Fig. 26 shows two cells. Green triangle symbols for 120° rotations, together with corresponding arc segments to indicate the angles as well, can be seen.

2.4.2 No. 14: $p3m1$ $(p3)$

What to do?

- **Select** from the left selection panel: Trigonal, point group 19, space group 156. Compare line 14 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

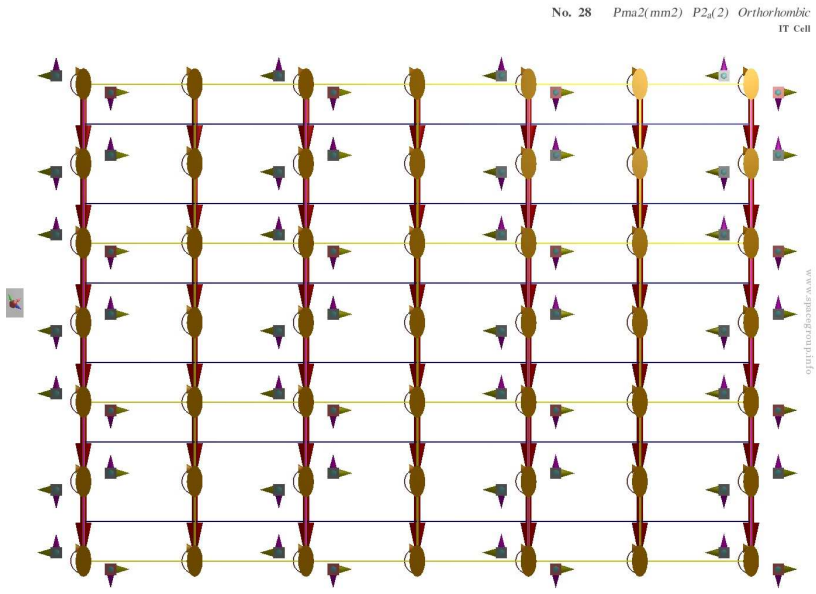

Figure 14: SGV view of 3×3 cells of 2D rectangular space group $p2mg$ $(p2)$.

Now one 2D cell of $p3m1$ appears, see Fig. 27. Fig. 28 shows two cells. Symbols for line of reflections (blue), glide reflection lines (yellow) with red arrows, and 120° rotations (green triangles) appear.

2.4.3 No. 15: $p31m$ $(h3)$

What to do?

- **Select** from the left selection panel: Trigonal, point group 19, space group 157. Compare line 15 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p31m$ appears, see Fig. 29. Fig. 30 shows 3×3 cells . Symbols for line of reflections (blue), glide reflection lines (yellow) with red arrows, and 120° rotations (green) appear.

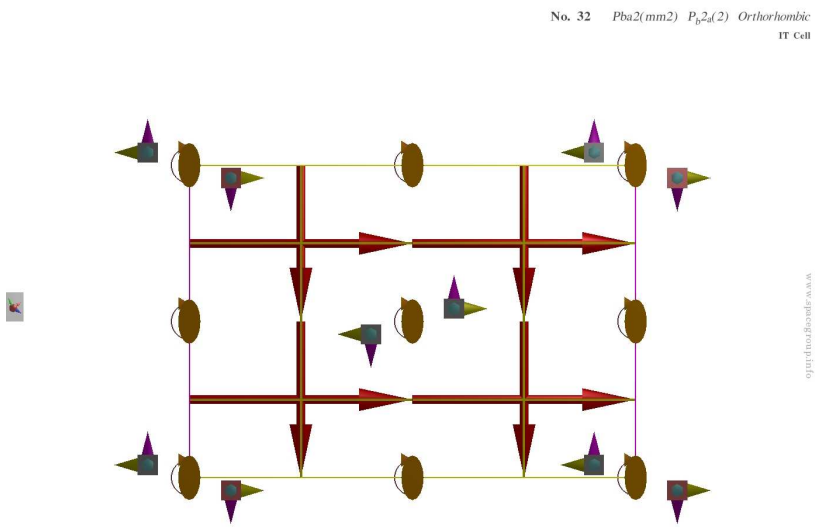

Figure 15: SGV view of 2D rectangular space group $p2gg$ (p_g2_g).

Tips for what else to do.

- Switching off the **cell/lattice frame** shows the horizontal and vertical lines of reflection clearly.

2.4.4 No. 16: $p6$ $(p\bar{6})$

What to do?

- **Select** from the left selection panel: Hexagonal, point group 21, space group 168. Compare line 16 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p6$ appears, see Fig. 31. Symbols for 60° (violet hexagons), 120° (green triangles), and 180° (orange ellipses) rotation centers appear.

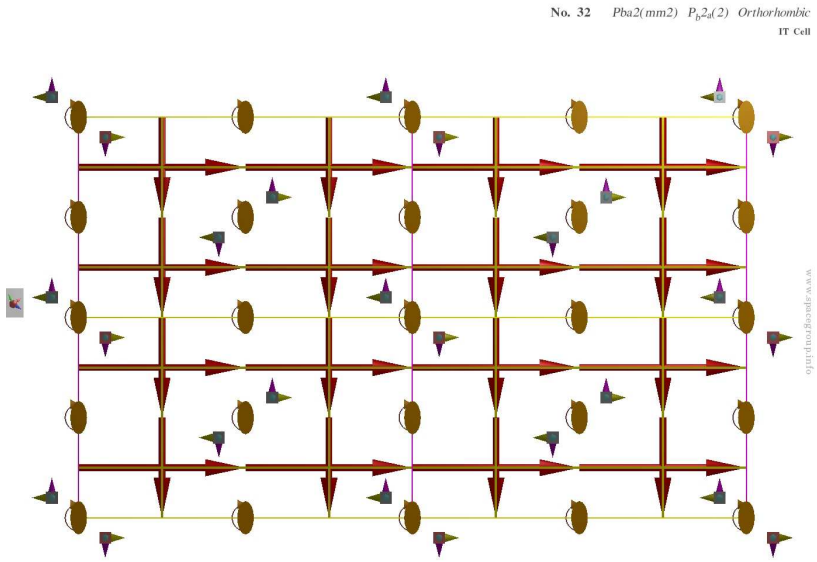

Figure 16: SGV view of 2×2 cells of 2D rectangular space group $p2gg$ (p_g2_g).

2.4.5 No. 17: *p6mm* (*p6*)

What to do?

- **Select** from the left selection panel: Hexagonal, point group 25, space group 183. Compare line 17 of lookup table Table 1.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of *p6mm* appears, see Fig. 32. Symbols for 60° (violet hexagons), 120° (green triangles), and 180° (orange ellipses) oration centers appear. Other symmetry symbols represent reflections (blue) and glide reflections (golden) with red arrows for the translation components.

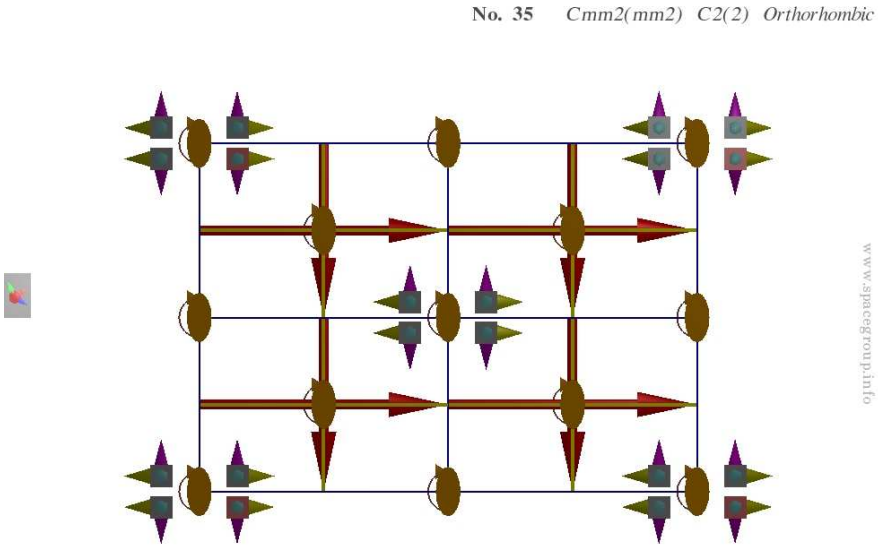

Figure 17: SGV view of 2D rectangular space group $c2mm$ $(c2)$.

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[3] H.S.M. Coxeter, *Discrete groups generated by reflections*, Ann. of Math. 35, pp. 588–621 (1934); H.S.M. Coxeter, W.O.J. Moser, *Generators and Relations for Discrete Groups*, Springer, 4th ed., 1980.

[4] E.Hitzer, C. Perwass, *Interactive 3D Space Group Visualization with CLUCalc and the Clifford Geometric Algebra Description of Space Groups*, accepted for Proc. 8th Int. Conf. on Clifford Algebras (ICCA8) and their Appl. in Math. Phys., 26-30 May 2008, Las Campinas, Brazil (2008).

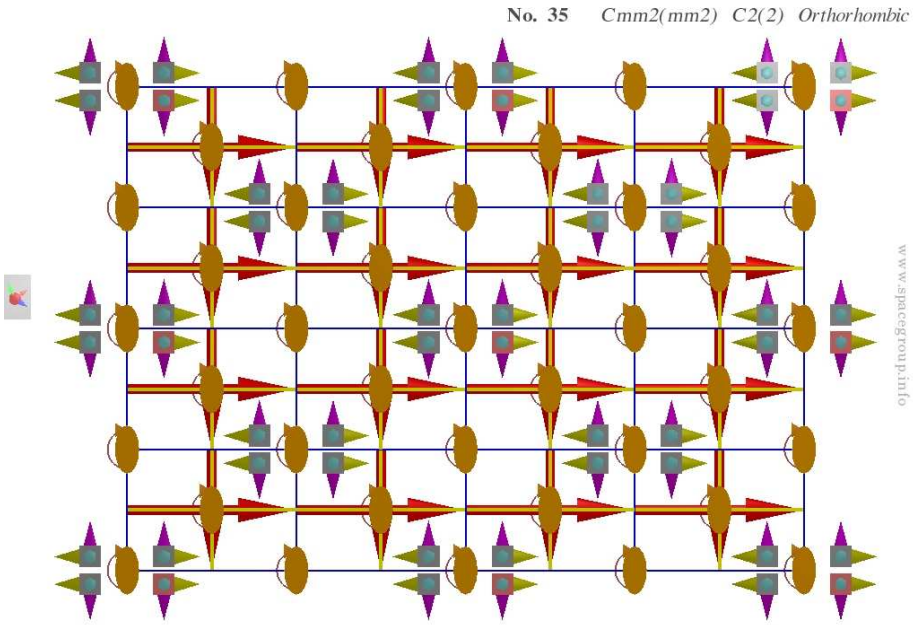

Figure 18: SGV view of 2×2 cells of 2D rectangular space group $c2mm$ $(c2)$.

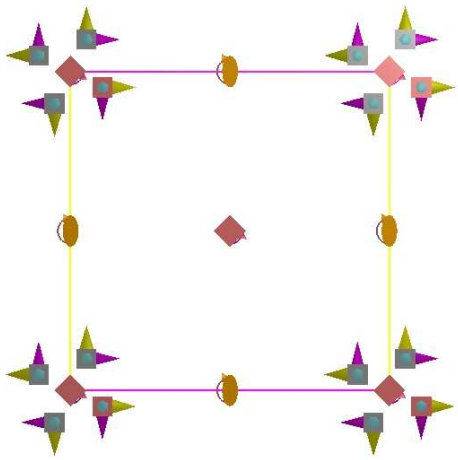

Figure 19: SGV view of 2D square space group $p4$ ($p\bar{4}$).

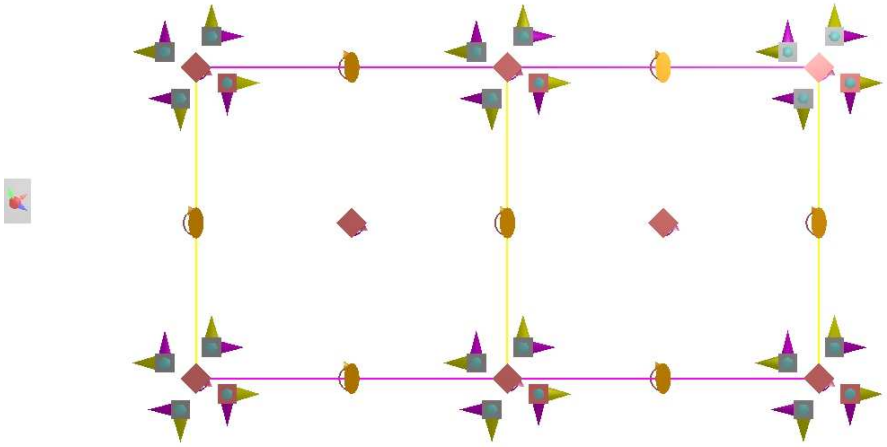

Figure 20: SGV view of two adjacent cells of 2D square space group $p4$ ($p\bar{4}$).

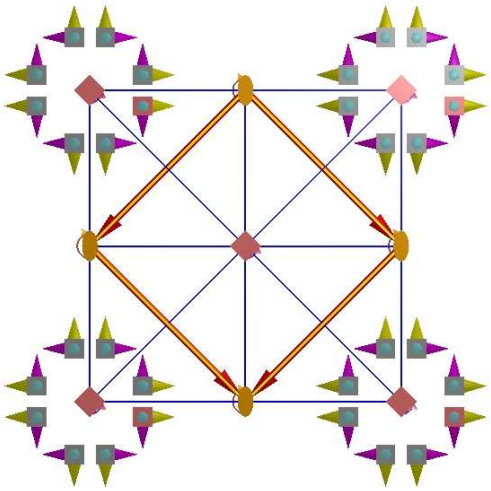

Figure 21: SGV view of 2D square space group $p4mm$ ($p4$).

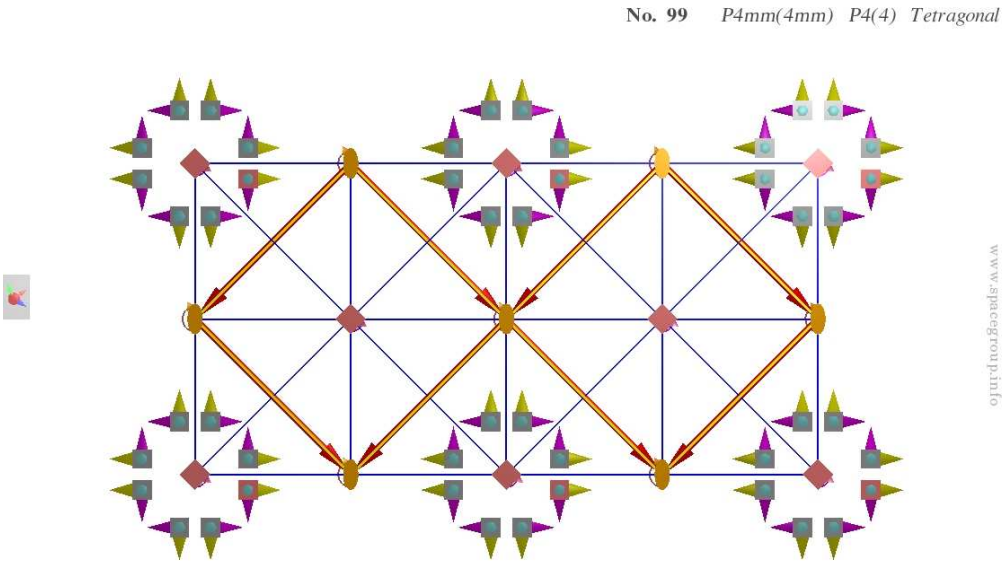

Figure 22: SGV view of two adjacent cells of 2D square space group $p4mm$ $(p4)$.

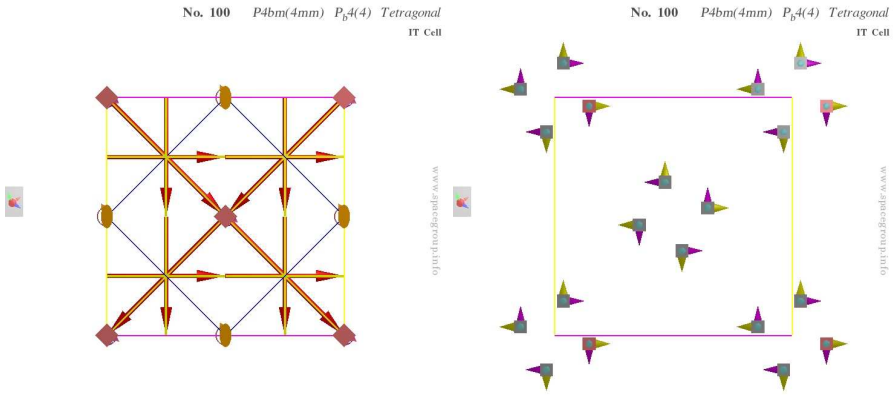

Figure 23: SGV view of 2D square space group $p4gm$ (p_g4). Left: Only symmetry elements, right: Only general elements.

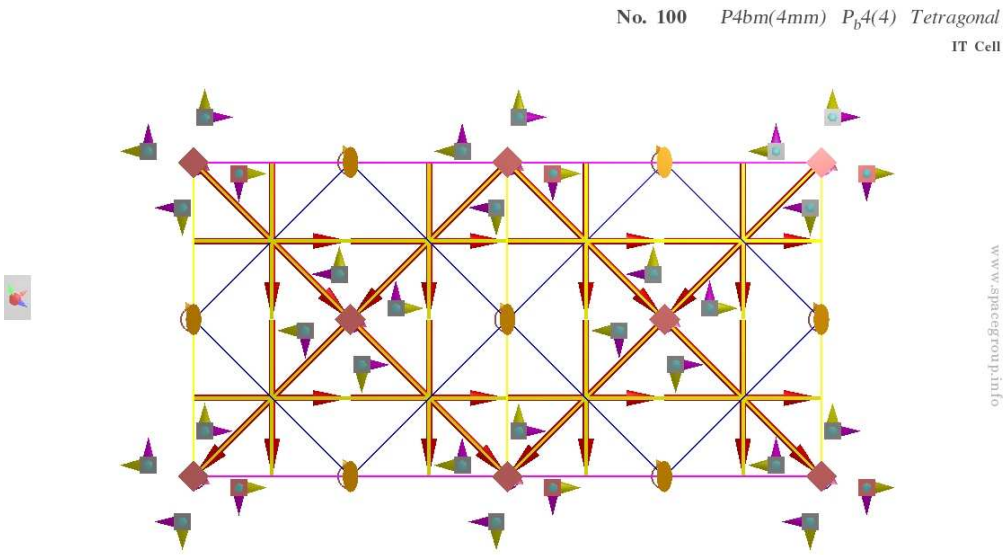

Figure 24: SGV view of 2 cells of 2D square space group $p4gm$ (p_g4).

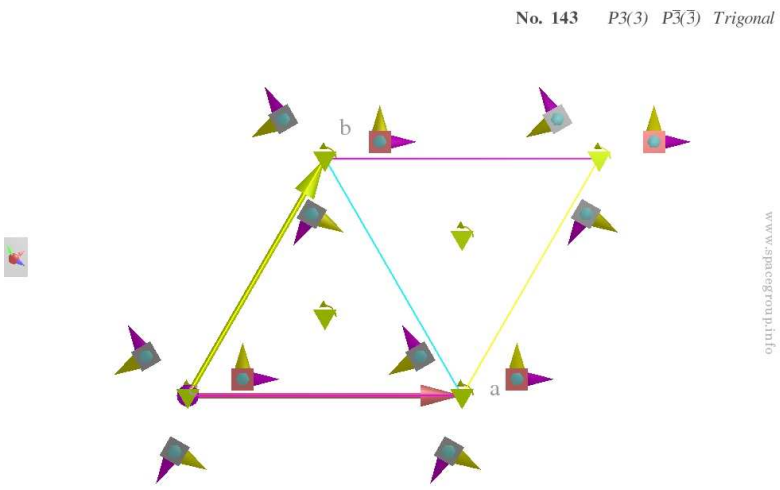

Figure 25: SGV view of 2D hexagonal space group $p3$ ($p\bar{3}$).

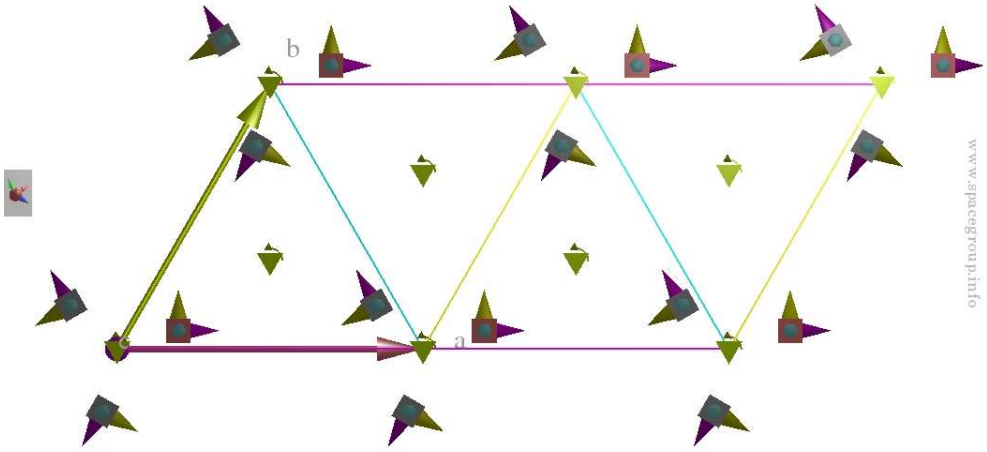

Figure 26: SGV view of two complete adjacent cells of 2D hexagonal space group $p3$ ($p\bar{3}$).

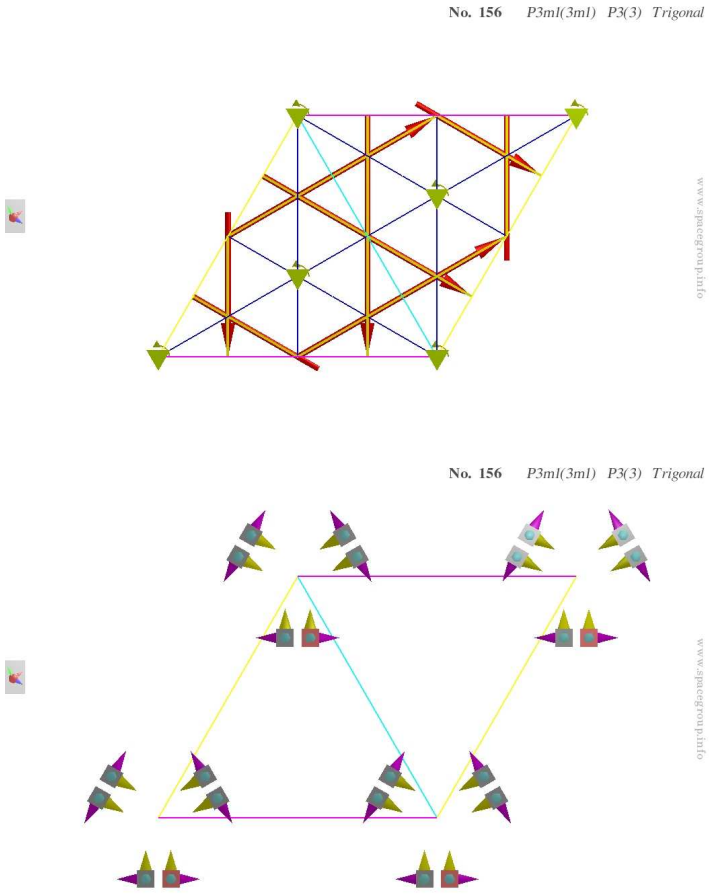

Figure 27: SGV view of 2D hexagonal space group $p3m1$ ($p3$). Top: Only symmetry elements, bottom: Only general elements.

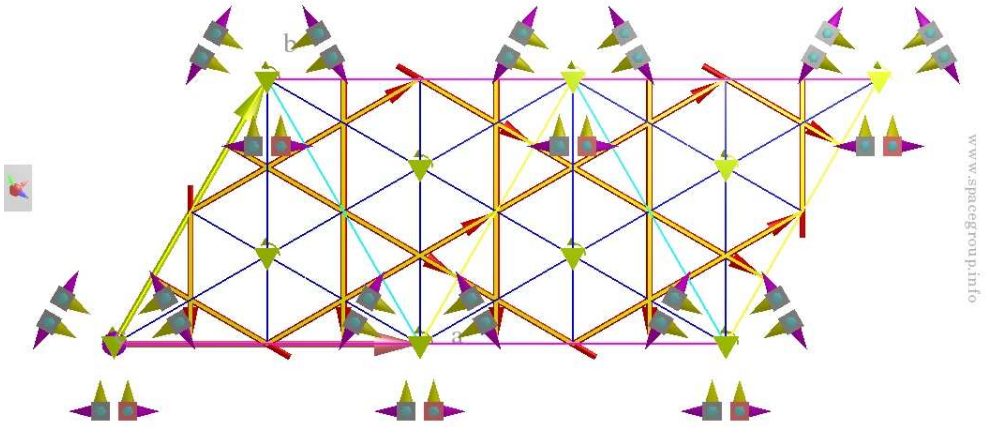

Figure 28: SGV view of two complete adjacent cells of 2D hexagonal space group $p3m1$ ($p3$).

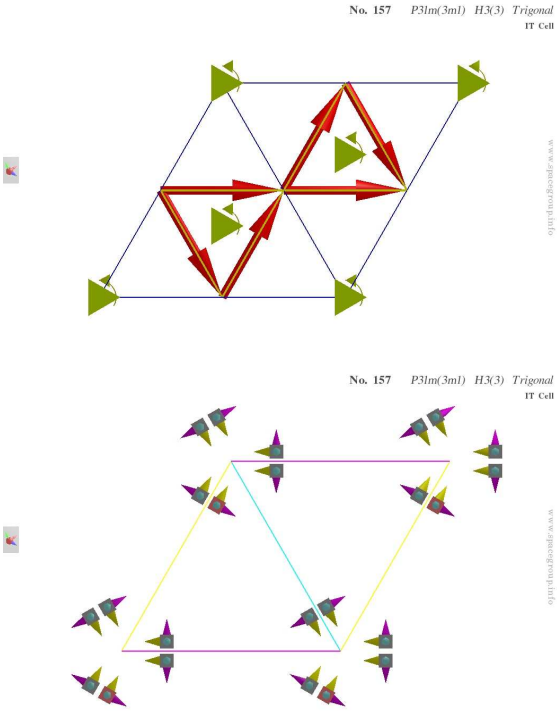

Figure 29: SGV view of 2D hexagonal space group $p31m$ $(h3)$. Top: Only symmetry elements, bottom: Only general elements.

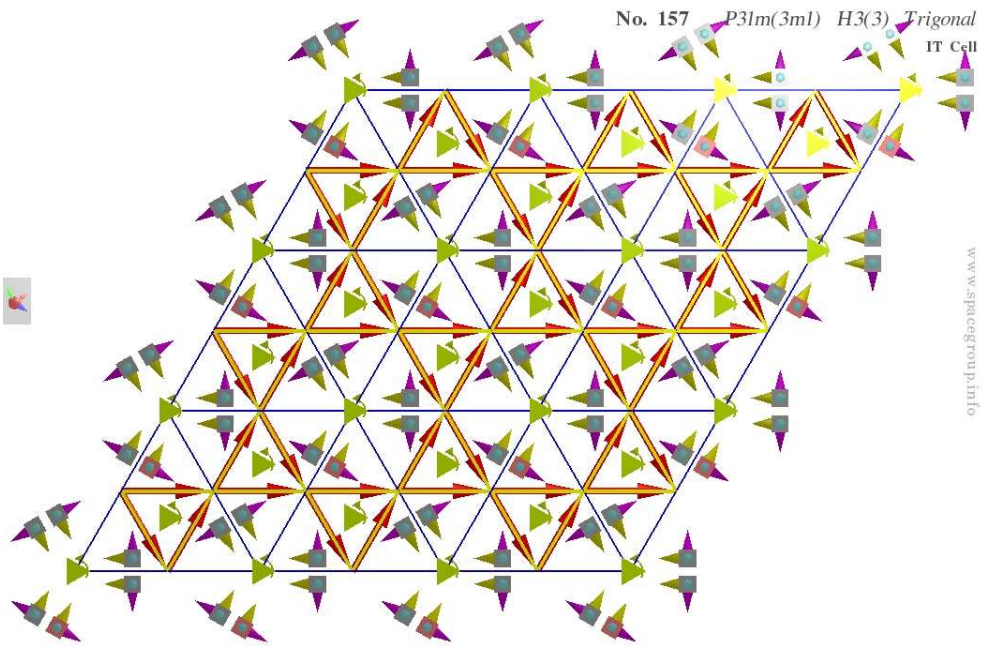

Figure 30: SGV view of 3×3 complete cells of 2D hexagonal space group $p31m$ $(h3)$.

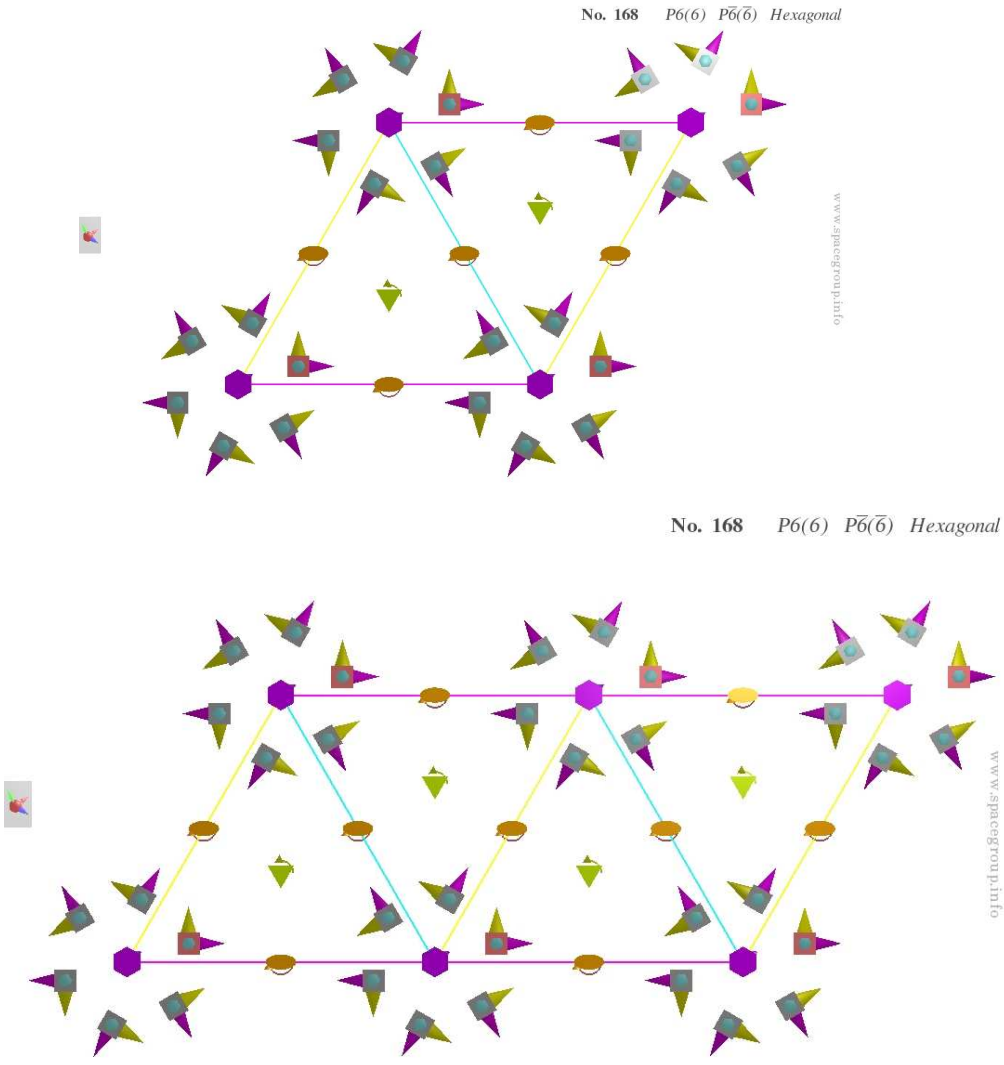

Figure 31: Top: SGV view of 2D hexagonal space group $p6$ ($p\bar{6}$). Bottom: SGV view of two complete adjacent cells of 2D hexagonal space group $p6$ ($p\bar{6}$).

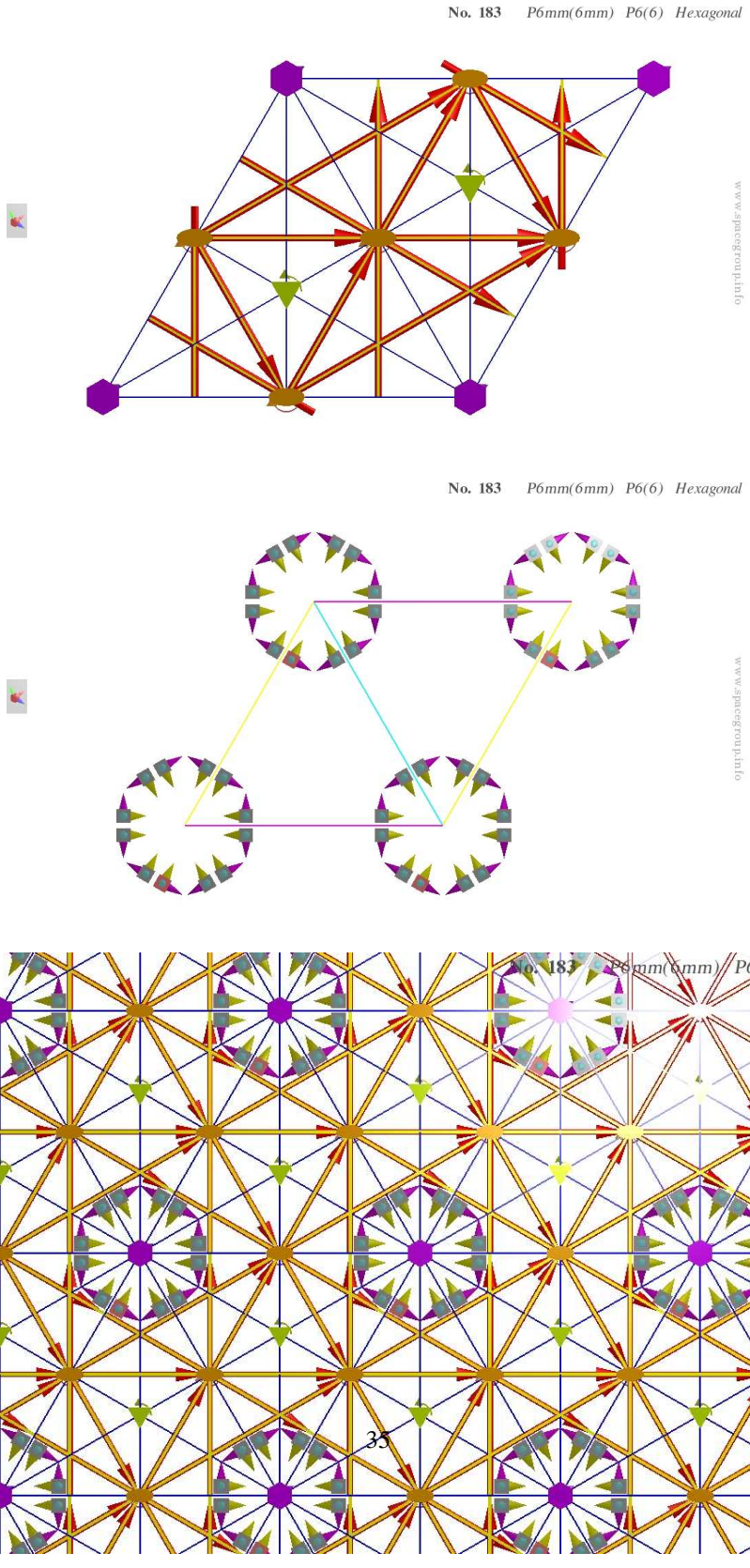

Figure 32: Top: SGV view of 2D hexagonal space group *p*6*mm* (*p*6). Bottom: SGV view of several complete cells of 2D hexagonal space group *p*6*mm* (*p*6).

[5] C. Perwass, *CLUCalc - a visual calculator*, www.clucalc.info

[6] C. Perwass, E. Hitzer, *Space Group Visualizer*, www.spacegroup.info (2005).

[7] The Space Group Visualizer can be purchased from Raytrix GmbH, www.raytrix.de