

INTERACTIVE VISUALIZATION OF PLANE GROUPS

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Fields of interest: Clifford geometric algebra, Crystallography, Neural networks, Elementary particle physics, Signal Processing (Christian Faith and Science, Education, Travel).

Publications: Perwass & Hitzer, 2005; Hitzer & Perwass, 2010.

Abstract: *This contribution shows how to successfully display the 17 two-dimensional space groups (wallpaper groups) in the interactive crystal symmetry software Space Group Visualizer (SGV) (Perwass & Hitzer, 2005). We show examples of four wallpaper groups that contain (as sub patterns, i.e as subgroups) all other 13 wallpaper groups. The SGV is described in (Hitzer & Perwass, 2010). It is based on a new type of powerful geometric algebra visualization platform (Perwass, 2000).*

The principle is to select in the SGV a three-dimensional (3D) super space group and by orthogonal projection produce a view of the desired plane two-dimensional (2D) space group. The choice of associated 3D super space group is summarized in the lookup table Table 1. The Section titles give the *Hermann-Maugin* (Hahn, 2005) and the *geometric* names (Hestenes & Holt, 2007) of the four selected wallpaper groups.

Plane group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Space group	1	3	6	7	8	25	28	32	35	75	99	100	143	156	157	168	183

Table 1: International numbers (Hahn, 2005) of 2D plane space groups (row 1), and of associated 3D space groups (row 2).

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 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 contribution uses white background pictures created with the SGV.

The SGV can be purchased (Perwass & Hitzler, 2005). The current instructions apply to version 2.2.5. (Coxeter 1934; Hestenes & Holt, 2007) describe the *Clifford geometric algebra* background of the software implementation.

1. WALLPAPER GROUP No. 7: $p2mg$ (p_g2)

What to do?

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

Now one 2D cell of $p2mg$ (geometric name: p_g2 , see (Hestenes & Holt, 2007)) appears, see Fig. 1 (left). Interactive rotation centers, lines of reflection symmetry (blue), and lines of glide reflection (yellow) with red glide vectors can be clearly seen.

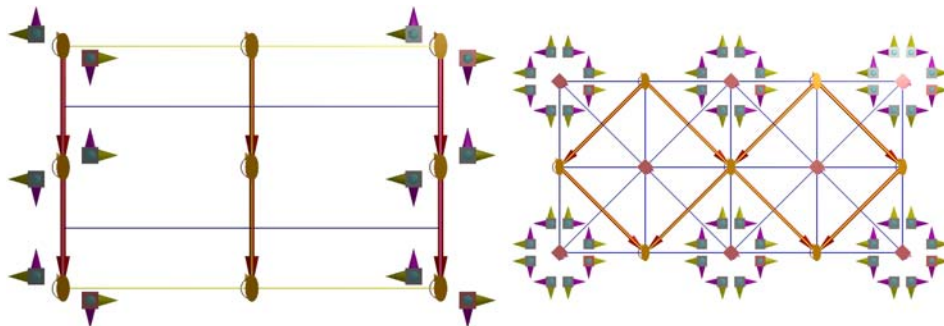


Figure 1: Left: 2D rectangular space group $p2mg$ (p_g2), right: Two adjacent cells of 2D square space group $p4mm$ ($p4$).

Tips for what else to do.

- Clicking on the **general element symbol** (colored cube-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. This shows the horizontal and vertical lines of reflection clearly.
- The **number of cells** in the a and b directions can be changed between 0 and 5.
- 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.

- 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 an interactive (orange) general element and then Shift+right mouse button held down, the **general element can be moved** up/down and left/right with the mouse. 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.
- Symmetries like reflection lines and glide reflection lines can be **subselected** by to orientation of their normal vectors, **location**, and **generator** expression.
- Additionally, the lines of glide reflection can be **subselected** by their **translation component**.

2. WALLPAPER GROUP No. 11: $p4mm$ ($p4$)

What to do?

- **Select** from the left selection panel: Tetragonal, point group 13, space group 99.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p4mm$ appears, see Fig. 1 (center). Fig. 1 (right) shows two cells. Interactive 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.

3. WALLPAPER GROUP No. 12: $p4gm$ ($pg4$)

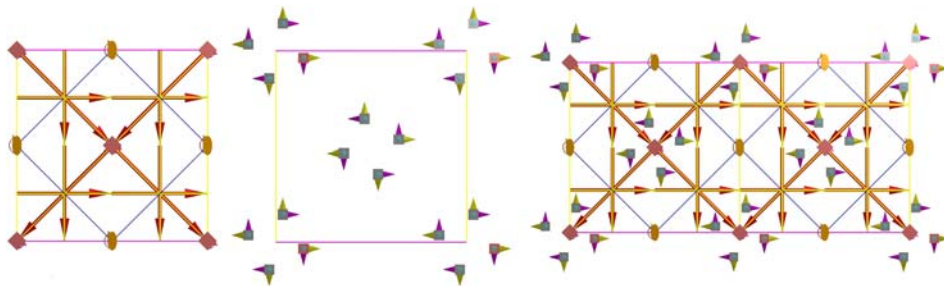


Figure 2: 2D square space group $p4gm$ ($pg4$). Left: Only symmetry elements, center: Only general elements, right: Two adjacent cells of 2D square space group $p4mm$ ($p4$).

What to do?

- **Select** from the left selection panel: Tetragonal, point group 13, space group 100.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p4gm$ appears, see Fig. 2 (left, center). Fig. 2 (right) shows two cells. Interactive symbols for lines of reflection (blue), lines of glide reflection (yellow) with red translation arrows, and for rotation centers (shape and color coded) appear.

4. WALLPAPER GROUP No. 17: $p6mm$ ($p6$)

What to do?

- **Select** from the left selection panel: Hexagonal, point group 25, space group 183.
- Drop down menu Visualization: Tick **Orthographic View (Ctrl+o)**.

Now one 2D cell of $p6mm$ appears, see Fig. 3. Symbols for 60° (violet hexagons), 120° (green triangles), and 180° (orange ellipses) rotation centers appear. Other symmetry symbols represent reflections (blue) and glide reflections (yellow) with red arrows for the translation components.

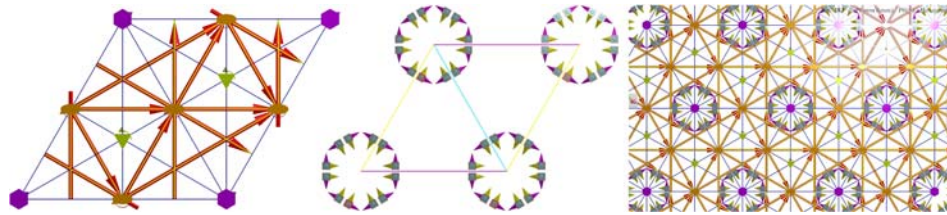


Figure 3: 2D hexagonal space group $p6mm$ ($p6$). Left: Only symmetry elements, center: Only general elements, right: Several complete cells.

The author thanks his dear family, C. Perwass, M. Aroyo and D. Proserpio. He acknowledges God the creator: *The fear of the Lord is the beginning of knowledge: but fools despise wisdom and instruction* (Salomon, ca. 950 BC).

References

- Coxeter H.S.M. (1934) *Discrete groups generated by reflections*, Ann. of Math. 35, pp. 588–621; Coxeter H.S.M., and Moser, W.O.J. (1980) *Generators and Relations for Discrete Groups*, Springer, 4th ed.
- Hahn, T., ed. (2005), *International Tables of Crystallography A*, Dordrecht: Springer. Online: it.iucr.org
- Hestenes, D. and Holt, J. (2007) *The crystallographic space groups in geometric algebra*, J.M.P. Vol. 48, 023514.
- Hitzer, E. and Perwass, C. (2010), Article, Accepted for Vaz, J., and Rodrigues, W. A., eds., *Interactive 3D Space Group Visualization with CLUCalc and the Clifford Geometric Algebra Description of Space Groups*, [Proc. of ICCA8, 26-30 May 2008, Las Campinas, Brazil].
- Perwass C. (2000) *CLUCalc - a visual calculator*, www.clucalc.info
- Perwass, C. and Hitzer, E. (2005) *Space Group Visualizer*, www.spacegroup.info (with free demo for space groups 1, 88, 230). The Space Group Visualizer can be purchased from Raytrix GmbH, www.raytrix.de
- Salomon, (ca. 950 BC), *Proverbs chapter 1 verse 7, King James Version of the Bible*, Oxford University Press.