

# GESUS, an Interactive Computer Application for Teaching and Learning the Space Groups of Symmetry

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## SM1. Program management (*How to use*)

1. Run the program (GESUS.exe) and wait until the main window of the program appears (the logo drawing disappears in a few seconds).

2. Press "Language" in the menu bar to choose the language.

3. Click <File> and <Open>. Then, two exercise types can be chosen: a) space group deduction using equivalent positions in the cell (a general coordinate "x,y,z" is used), then choose <SG by general position>; or b) space group deduction using the SG full Hermann–Mauguin symbol, then choose <SG by name>.

4. A window appears where the user must choose the folder with the list of proposed exercises (exercises folder), from which one of them should be selected. Currently, GESUS v.2.4 includes 74 space groups of symmetry for Triclinic, Monoclinic, and Orthorhombic.

5. The preselected origin is shown at the top of the grey area of the main window. In addition to the representation of the motifs corresponding to the exercise chosen in the white drawing window, the empty cell is displayed, and the notation of the selected space group is indicated on the right-hand side, according to the type of exercise previously chosen.

In the drawing windows, a grey mesh "cell" is displayed as background, which will be used as a template on which the symmetry elements to be drawn will be arranged. The intersections of the lines of this mesh constitute "sites", and there is an "extra site" in the upper left corner of the drawing window (the symmetry elements will be drawn in these "sites").

In case the general position option has been selected, the atoms/motifs are drawn on a general arrangement determined by their three-dimensional coordinates x, y, and z, so that the flat drawing itself represents the coordinates x and y, while the 3D height or depth is represented by the corresponding z coordinate (text next to the motif).

The motifs are graphically displayed as circles with white fill ("left" positions), black fill ("right" positions), and semi-black-white fill ("left" and "right" positions with different heights).

6. Select a symmetry operator from among the 32 buttons on the left side of the drawing window. Information (drawing and text) about the selected element will appear at the top of the window.

7. When the cursor is positioned over the drawing window, it becomes a cross, and when placed near any "site", it will represent the symmetry element selected in the drawing window if the left mouse button is pressed.

All elements necessary to complete the current exercise will be placed in their corresponding positions. If an element is attempted to be placed in an incorrect position, a warning window appears.

Pre-drawn symmetry elements can be selected/deselected by simultaneously pressing the <Control> key on the keyboard and the left mouse button.

To delete a pre-drawn operator, select it by <Control + left mouse button> and then press the <Del> key on the keyboard.

To assign a specific “z” coordinate to a symmetry operator, select the element by pressing <Control + left mouse button>, and then press the corresponding “z” coordinate (<1/4>, <1/8>, or <3/8> button).

Successful selection of the compatible elements of symmetry with the disposition of the motifs/atoms in each group requires prior knowledge of symmetry theory (see bibliography).

8. Once the drawing exercise of all existing symmetry elements has been completed, press the <Continue> button.

9. If the type of exercise of general positions has been performed in the window that appears in the upper-right part, select the crystalline system to which the exercise corresponds. In this version, only triclinic, monoclinic in two settings, and orthorhombic systems are available.

10. Once the System, a new window, appears, the user must select the compatible crystal class with the proposed exercise (previous knowledge of symmetry theory is required).

11. Once the Crystal class, another window, appears, the user must select the SG obtained as a solution to the drawn elements (previous knowledge of symmetry theory is required).

12. Once the SG is set, the <Correct> button appears. Click this button, and the exercise will be evaluated. A pop-up window appears indicating that the score obtained from the solutions drawn emerges.

If the score is 10.00 points, the exercise is completed and correct. Click the <Accept> button. Now, the options are: to start a new exercise, to save the generated image, or to exit by the <File> menu.

If the score does not reach 10.00 points, it is also important to press the <Accept> button. Wrong System, Crystal class, or SG will appear indicating the corresponding error in a new pop-up window. Subsequently, another window will specify erroneous symmetry elements, which will be marked in red. The missing position of the elements will appear in blue. They are automatically selected. Clicking the <Del> key will delete the entire selection and allow the exercise to continue until it is completed. Pressing the left mouse button on the grey area, instead of pressing the <Del> button, will cause the missing elements to disappear (blue), but the elements that are wrong (red) will remain selected.

## **SM2. Resolving an SG exercise using GESUS v.2.4. (an example)**

### *SM2.1. Resolving SG by the general position of motifs*

The following instructions describe how to correctly complete exercise number 30 for SG Pnc2 (orthorhombic) by general position.

1. Open GESUS software.

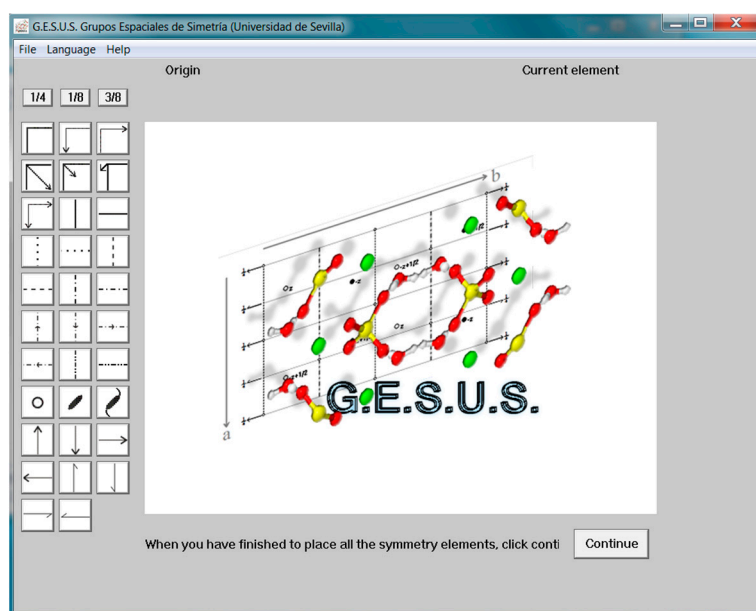


**Figure S1.** GESUS v.2.4. user graphical interface.

2. Go to File -> Open -> SG by general position.

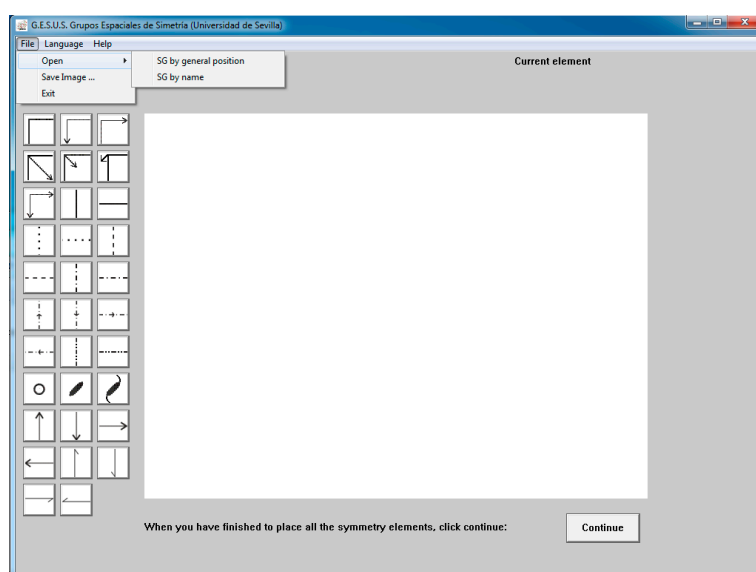


**Figure S2.** Open a file in GESUS v.2.4.

3. Look for the folder that contains the exercises and choose an exercise file, such as number 30 (30.sgf).

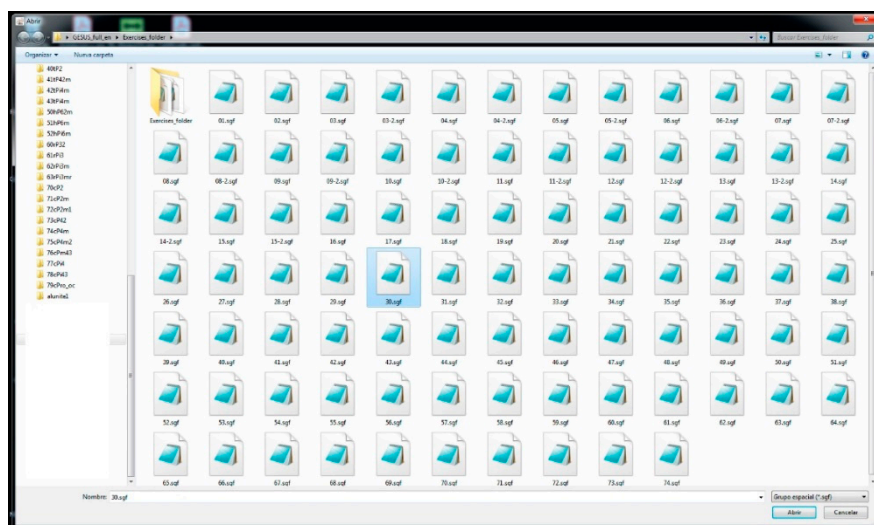


**Figure S3.** Exercise files in GESUS v.2.4.

4. The drawing window shows a pattern with black and white motifs (opposite motifs and z-coordinate). Look at the white motifs on the top left and the black motifs on the right (on top) with  $z+1/2$ ; between both motifs there is a c-glide plane according to (010). Choose the c-glide plane (click on the icon) and select the right position.

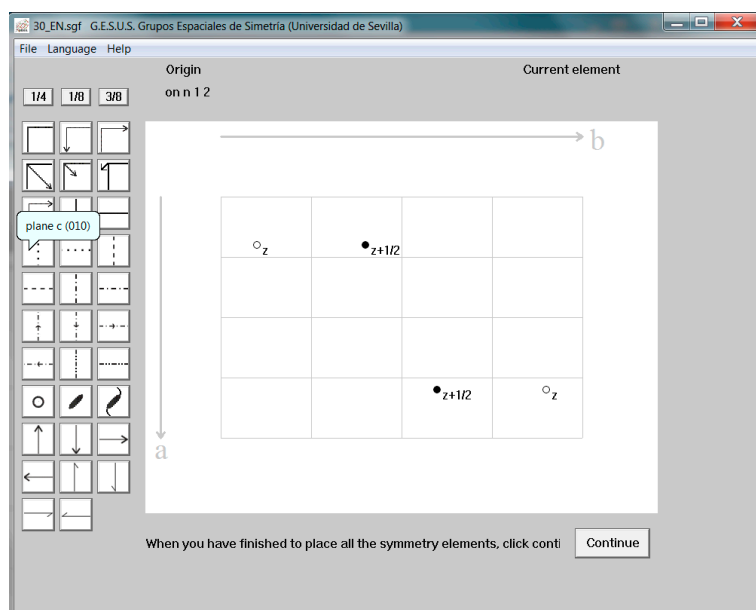


**Figure S4.** Drawing window in GESUS v.2.4.

5. Choose the c-glide plane (click on the icon) and select the right position.

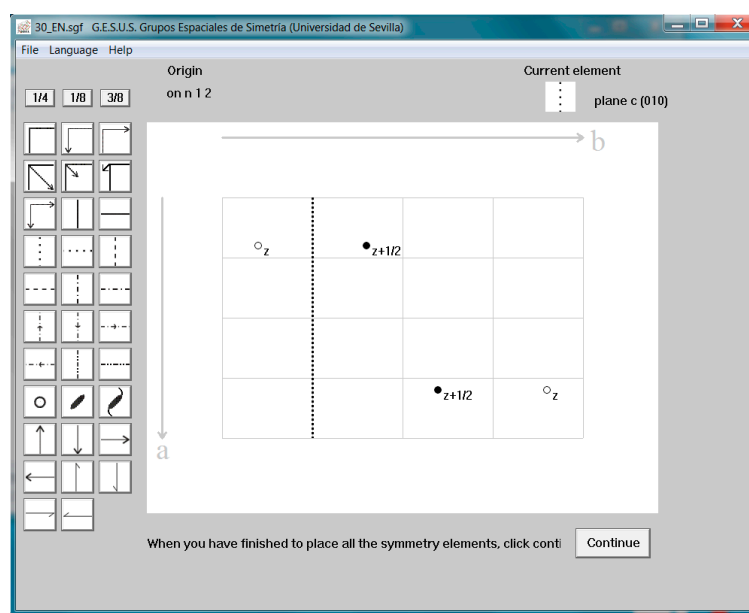


**Figure S5.** Drawing a c-glide plane in GESUS v.2.4.

6. Applying the combination of a reflection and perpendicular translation, another c-glide plane must be between the bottom-right motifs.

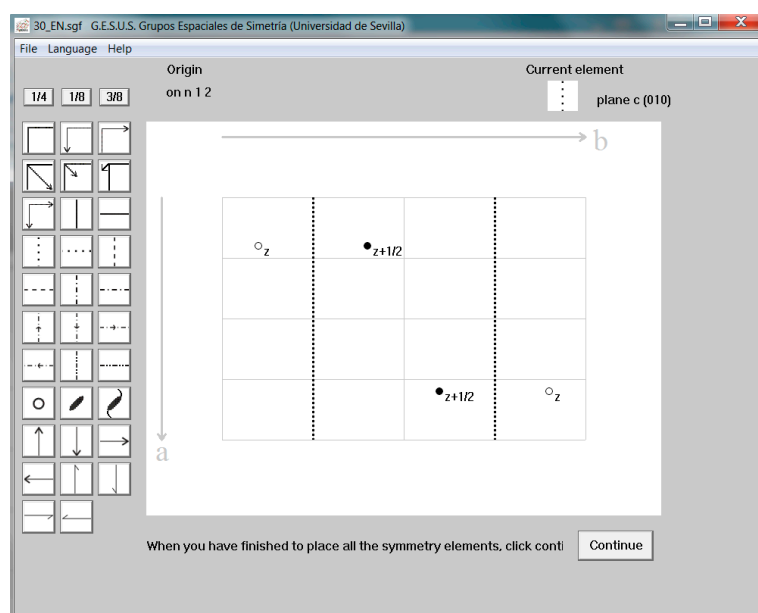


**Figure S6.** Drawing another c-glide plane in GESUS v.2.4.

7. Look at the white top-left and black bottom-right motifs, the corresponding symmetric element is a slide plane type 'n' according to (100). Choose and place it in the middle of the pattern and the corresponding combination.

8. Finally, look at the relationship between equivalent white motifs (or black motifs), the two-fold rotation axis in [001] located in the middle.

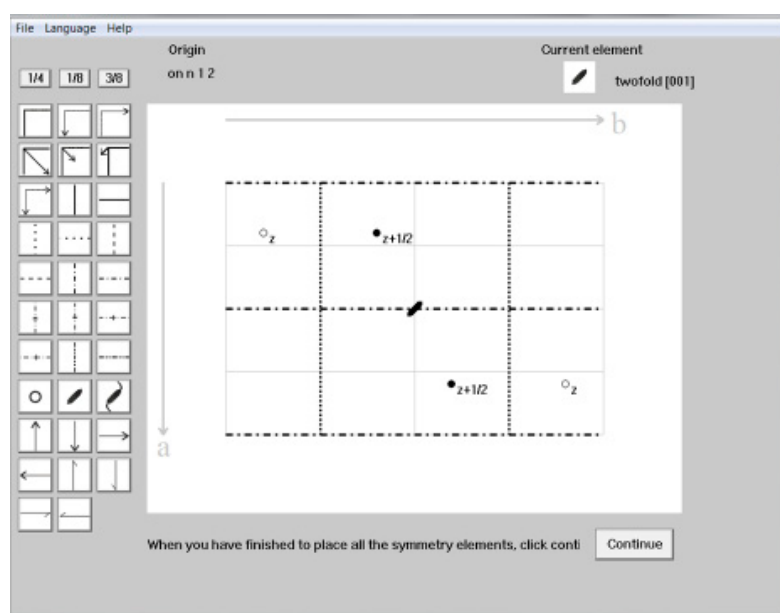


**Figure S7.** Drawing a two-fold rotation axis in GESUS v.2.4.

9. Apply the combination of a twofold axis with perpendicular translation, generating a new twofold axis compatible with the distribution of existing motifs.

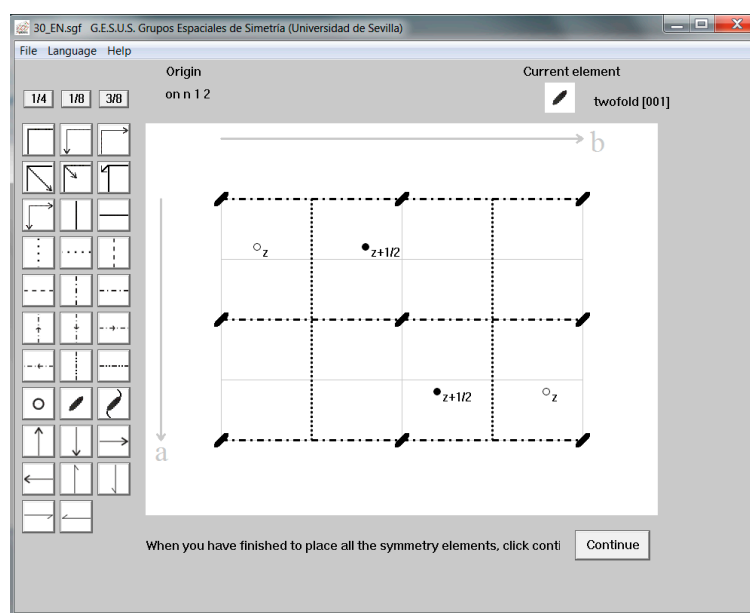


**Figure S8.** Drawing of the completed symmetry elements in GESUS v.2.4.

10. Click <Continue> and choose the Crystal system from the pop-up menu. In this case, the crystal system is orthorhombic.

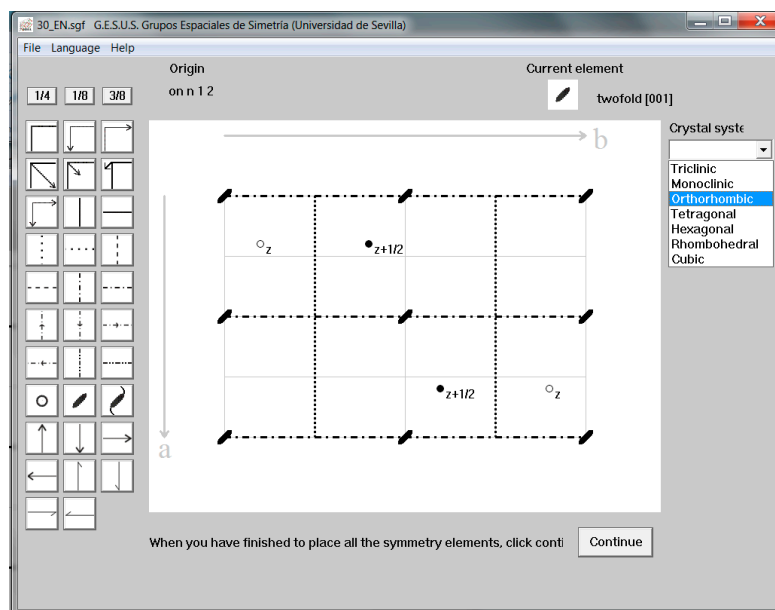


**Figure S9.** Choosing the Crystal system in GESUS v.2.4.

11. Choose the Crystal class from the new pop-up menu. Now, it is 2mm.

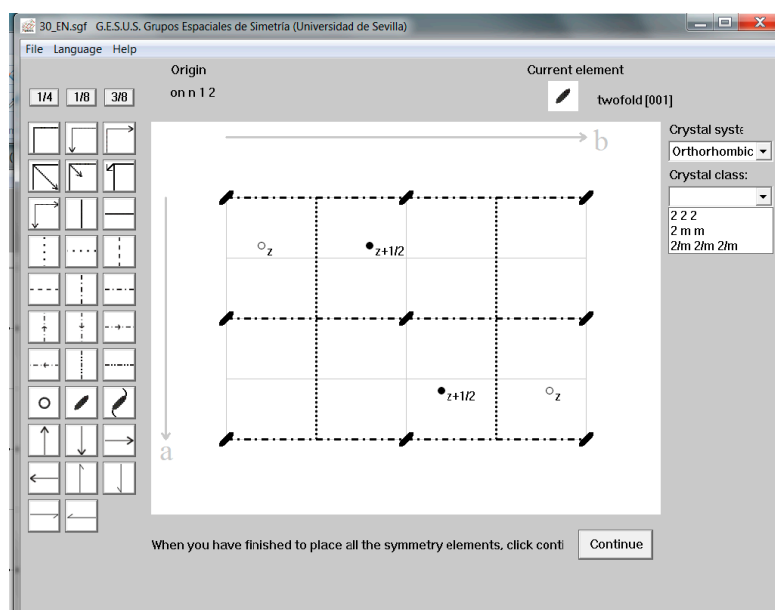


**Figure S10.** Choosing the Crystal class in GESUS v.2.4.

12. Select the corresponding space group. Here, it is Pnc2.

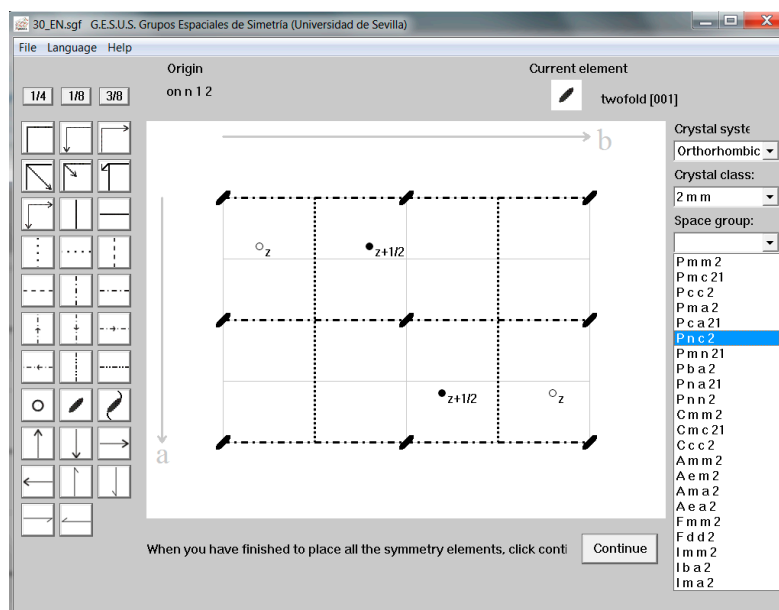


**Figure S11.** Choosing the space group in GESUS v.2.4.

13. Click the <Correct> button: the new window shows the final mark of the completed exercise.

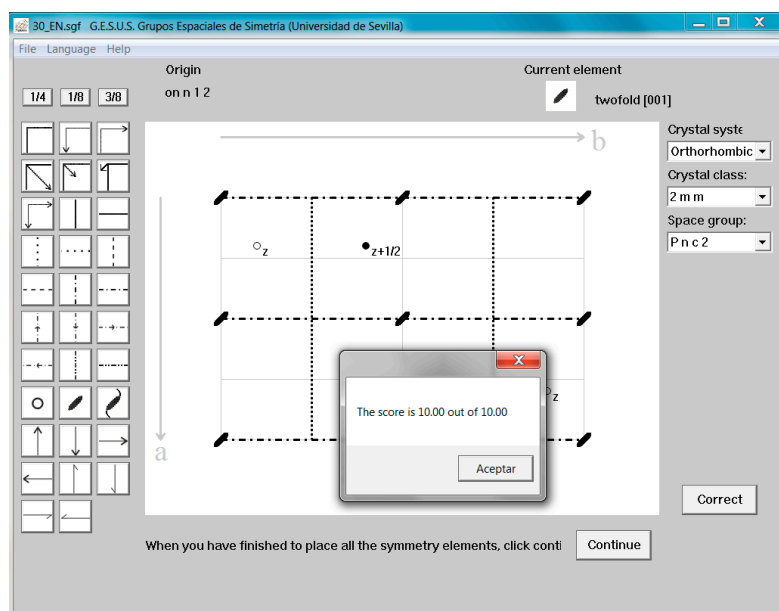


**Figure S12.** The completed exercise in GESUS v.2.4.

### SM2.2. Resolving SG by name

The following instructions describe how to complete the same exercise number 30 for SG Pnc2 (orthorhombic) using the option to resolve by name. The sequence is similar, but instead of using the position of motifs for the resolution, the SG name in Hermann–Mauguin notation is used as a reference. In Step 2, described above, it will be clicked via File -> Open -> SG by name instead of SG by general position (the exercise files remain the same).

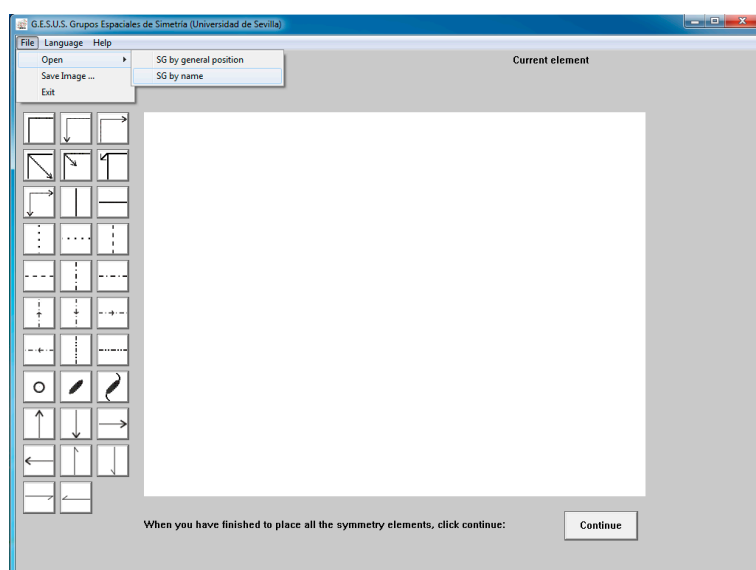


**Figure S13.** Opening an SG file by name in GESUS v.2.4.

The drawing window shows the reference grid pattern, and the name of the SG is displayed in the top-right corner.

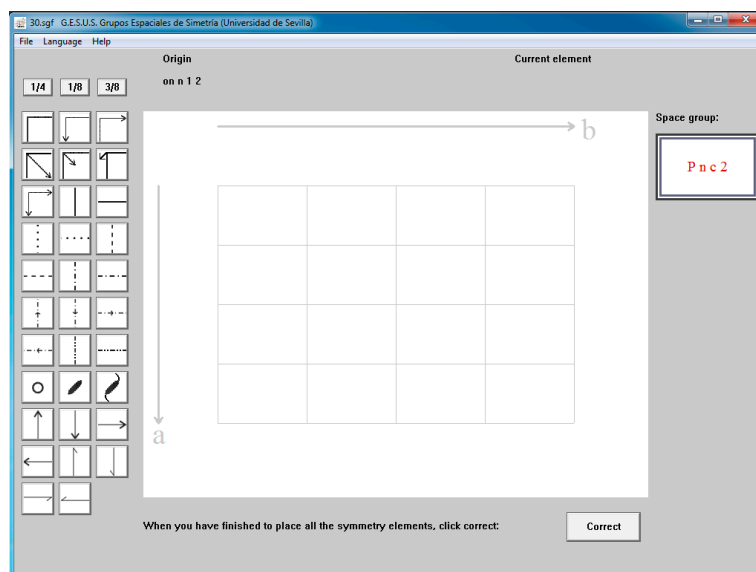


**Figure S14.** Drawing window for SG by name resolution exercise in GESUS v.2.4.

The symmetry elements necessary to correctly complete the exercise will be selected.

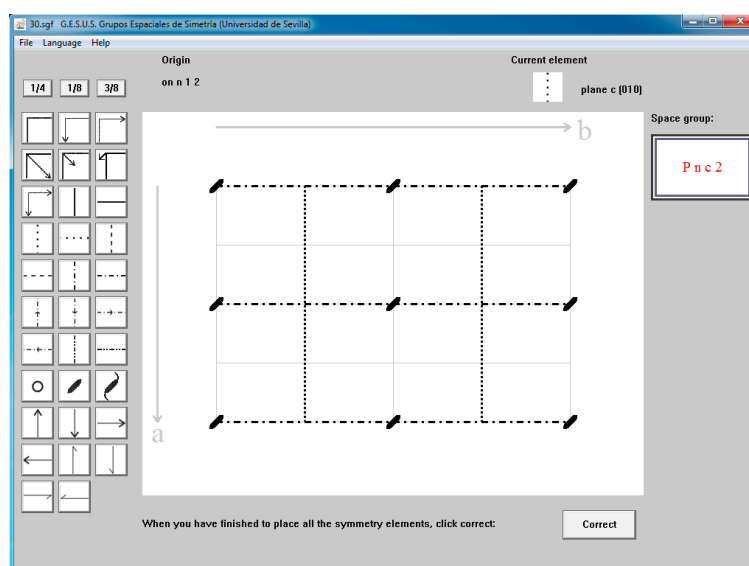


**Figure S15.** Drawing of the completed symmetry elements in GESUS v.2.4.

Finally, click <Continue> and a new window shows the last mark of the completed exercise.

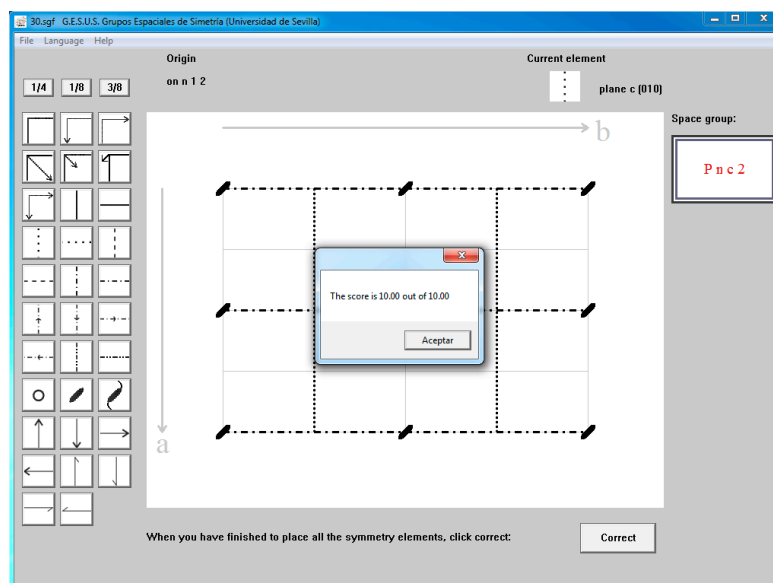


**Figure S16.** Completed SG exercise by name in GESUS v.2.4.