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

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Abstract: This paper describes a digital application designed for learning Space Groups of Symmetry (SGS). It teaches how to recognize the operations performed by the symmetry elements, both point (or 2D) operators (proper and improper rotations, including mirroring, inversion, and other rotoinversions), and space (or 3D) operators (screw axes and glide planes), as well as their combinations with the translations of the lattice. The software applies a 3D space vision to identify the elements of symmetry compatible with the proposed structural models. The symbols of internationally accepted representation are used. The system, class, and space group of the crystal that agree with the proposed model are solved. Two settings are taken into account in the Monoclinic system. The application self-evaluates and assesses the knowledge acquired, allowing each exercise to be re-done until it is correctly completed with the appropriate recommendations. This application constitutes a useful and easy-to-use tool for SGS learning. It is aimed at beginner students of crystallography, with elementary knowledge about elements of symmetry, Bravais lattices, crystal classes, and wallpaper groups.

Keywords: chemistry; geological science; condensed matter physic; symmetry properties; crystallography; Space Groups of Symmetry; computer-aided crystallographic teaching

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1. Introduction

Knowledge of crystalline structures and their symmetry properties is essential for understanding the implications derived from the physical and chemical properties of most solids. Some symmetry operators significantly contribute to the lattice energy calculated for the crystal structures of organic molecules [1] and other physical properties [2,3]. The symmetry operations are very important for the study of the physical properties of a crystal, since they must include the symmetry operations of the point group of a crystal [4]. Moreover, symmetry is used as a fundamental property of the orderly arrangements of atoms found in crystals, as it characterizes the external well-formed crystals, identifies repeating patterns of molecules, and simplifies both data collection and nearly all calculations.

In order to perform structural determinations, a Space Group of Symmetry (SGS) must first be assigned. When the structural data of a compound are described in the literature, the space group symbol, unit cell dimensions, and coordinates "x, y, z" for the atoms are provided. For this reason, curricula with topics related to crystalline matter (Chemistry, Materials Engineering, Geology, Condensed Matter Physics, etc.) usually include subjects such as Crystallography, in which space symmetry is taught.

There are numerous didactic resources on the internet dedicated to Crystallography, including applications (apps) and programs that the authors have developed to facilitate the understanding of different concepts [5–13]. Even point groups [14–16] and space groups [17] are displayed graphically. Nevertheless, to the best of our knowledge, there are no applications that interactively teach how to deduce the position of each symmetry element using the "international standard" space group diagram (the main difference from the above-mentioned software or applications), either by taking into account the arrangement of motifs or combinations of symmetry operators. It is to be understood as an international standardized space group diagram, as the symmetry element diagram displays the location and orientation of the symmetry elements of the space group. Those diagrams are orthogonal projections of the space-group unit cell onto the plane of projection along a basis vector of the conventional crystallographic coordinate system.

2. A Crystallographic Overview and Its Implications for GESUS

Crystal structures are classified according to their symmetry properties. To do this, information about the symmetry of the crystal pattern is extracted through crystallographic models that simplify the repetition of atoms, ions, or molecules and complete the description of the symmetry by studying the arrangement of the motifs in each lattice cell. The GESUS application has been designed to help students and enthusiasts follow this methodology.

A space group is the set of symmetry operators (and respective operations or isometries) that completely describe a 3D periodic pattern or a crystal arrangement of atoms. A symmetry operation on a given object is an isometry and leaves the object invariant (as a whole) [18]. The distances and angles between each point of the object are kept by the transformation. These symmetry operators are used in GESUS for the implementation of symmetry operations.

The 230 space groups are combinations of the 32 crystallographic point groups and the 14 Bravais lattices, considering that the combination of point symmetry operators and translations generates new symmetry operators (glide reflections and screw rotations) (Table 1). The symbols of the symmetry operators used in GESUS v.2.4 are shown in Tables 2 and 3.

The GESUS application allows the user to perform two types of exercises. The first one consists of selecting symmetry operators from a menu and placing them in a graphical interface according to the position of the motifs (small black or white circles depending on their handedness as chiral objects) (Figure 1). In the second case, the Hermann–Mauguin notation of an SGS is given and the corresponding symmetry operators have to be selected instead of showing the motifs (see Supplementary Materials).

Table 1. Symmetry operators used on space groups [1].

Symmetry Element	Geometry	Operation
Mirror plane "m"	planes	reflection through plane
Glide plane "a, b, c, n, d, e"	planes	glide reflection through plane and a lattice-translation vector
Rotation axis "n"	line	rotation around line, angle 2p/n, n = 2, 3, 4, or 6
Screw axis "n_j"	line	Screw rotation around line, angle 2p/n, j/n time shortest lattice translation along line, right-hand screw, n = 2, 3, 4 or 6, j = 1, . . . (n − 1)
Rotoinversion axis	line and point on line	rotation around the line, angle 2p/n, followed by inversion through the point, n = 3, 4, 6
Centre	point	inversion through point

[1] Modified form [19].

Table 2. Rotations, screw axes, and their symbols used in GESUS v.2.4.

Printed Symbol	Symmetry Axis	Graphic Symbol	Nature of the Screw Translation [1]
1	Identity	none	none
−1	Inversion	o	none
2	Rotation diad or twofold rotation axis	(⊥ paper) (// paper)	none
2_1	Screw diad of twofold screw axis	(⊥ paper) (// paper)	c/2 a/2 or b/2

[1] "a, b, c" lengths of the unit.

Table 3. Symmetry planes and their symbols used in GESUS v.2.4.

Printed Symbol	Symmetry Plane	Graphic Symbol: Normal to Plane of Projection	Graphic Symbol: Parallel to the Plane of Projection	Nature of Glide Translation [1]
m	Reflection plane (mirror)			None
a, b	Axial glide plane			a/2 or b/2
c			none	c/2
n	Diagonal glide plane (net)			(a + b)/2 or (b + c)/2 or (a + c)/2
d	"Diamond" glide plane		3/8 1/8	(a ± b)/4 or (b ± c)/4 or (a ± c)/4
e	"Double" glide plane			(a/2 + c/2) or (b/2 + c/2) or (a/2 + b/2)

[1] "a, b, c" lengths of the unit.

In the first type of exercise, once all the symmetry operators are drawn from the motif positions, the user must indicate the crystal system, the crystal class (point group), and, finally, the name of the space group. Then, GESUS provides different possibilities in pop-up menus (Figure 2).

Interpreting space group symbols requires prior knowledge of the crystal system. This means knowing the type and symbols denoting the Bravais lattice and the orientation of symmetry operators.

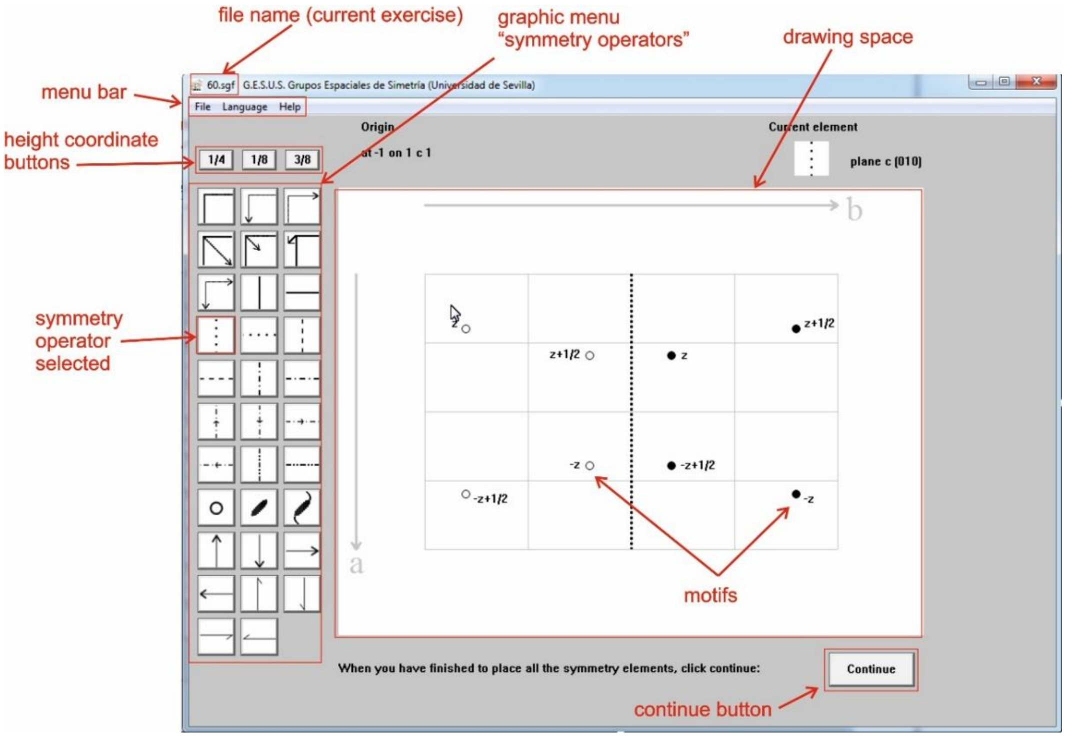

Figure 1. General view of the GESUS v.2.4 interface.

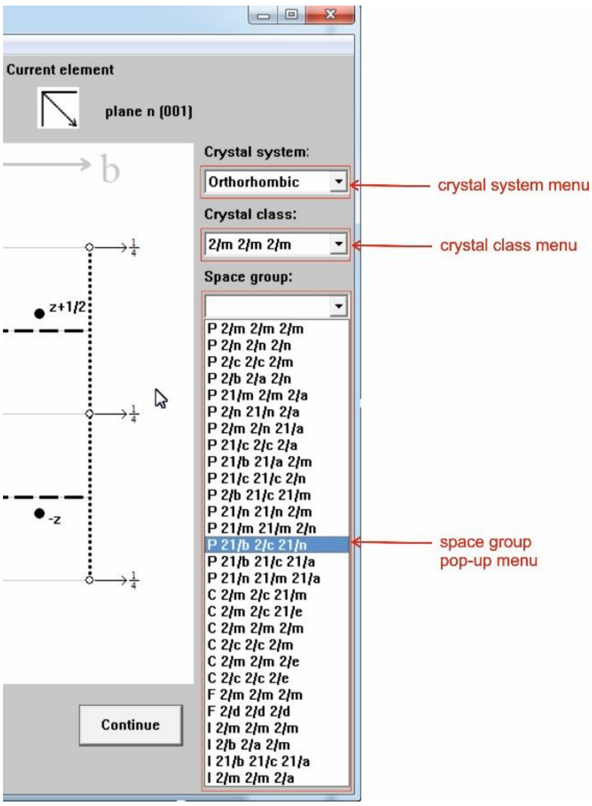

Figure 2. System, class and Space Groups pop-up menu.

3. Objective, Motivation, and Significance

The main aim of GESUS is to offer a useful and easy-to-use tool to teach and learn the space groups of symmetry using space group diagrams from the International Tables for Crystallography [18].

In addition, this tool will allow us to develop competencies such as:

(a) Teaching one to recognize the operations carried out by the symmetry operators and their combinations with the lattice translations.
(b) Recognizing and using symbols to represent symmetry operators, according to their arrangement in space, in representations projected on the “a-b” plane.
(c) Identification of the crystal system, crystal class (point group), and space group (Hermann–Mauguin international notation) from the operators that have been graphically drawn.
(d) Solving problems related to conventions that are usually used by agreement (e.g., the imposition of an origin, different settings in the monoclinic system, etc.).

The main motivation behind studying space groups is to acquire the ability to sort crystal structures according to their symmetry properties. As many properties of a structure can be derived from its group of symmetry, GESUS allows for the simultaneous investigation of the properties of several structures.

In general, SGS teaching entails numerous difficulties derived from the scarce space vision of students and the complexity displayed by some combinations of symmetry operations (especially when translations are included).

According to previous studies [20,21], visualization skills can be improved by appropriate training in a 2D environment that includes the features of a 3D interaction since the interactivity in these 2D-3D environments is useful for the user’s spatial understanding [20].

How can knowledge about space groups be taught at the undergraduate level when resources and student background knowledge are often limited? Even more important, how can the maximum number of students be engaged in these learning activities? Answers can be found in part in the pedagogical approach [21] and the careful construction of learning activities such as the GESUS application.

Nowadays, students show great aptitude for using computer applications, especially if they are free and have a structure similar to games played for entertainment. This software encourages the acquisition of knowledge through self-evaluation and self-correction. GESUS can also be very useful for teachers, who could easily follow the evolution of learning in the virtual teaching platforms provided by many universities.

4. Target Users

Crystallography applications do not have to only serve chemistry graduate programs; for instance, they can often be found in geology and material science programs [22]. Rossi and Berman [23] noted that, while it is important to teach the fundamentals of crystallography to beginning science students, the study of crystallography has largely been neglected.

GESUS was designed to be used even by users inexperienced in the fine details of combinations of symmetry operations. Several pop-up help windows are included, which appear when the crystal system, class system, or space group are wrong. Another pop-up help window is shown if the locations of one or more symmetry operators are performed incorrectly or are missing. GESUS also provides an automatic score that marks the exercise done (Figure 3), allowing users to correct mistakes and reach the maximum score of 10.00 (100% correct exercise).

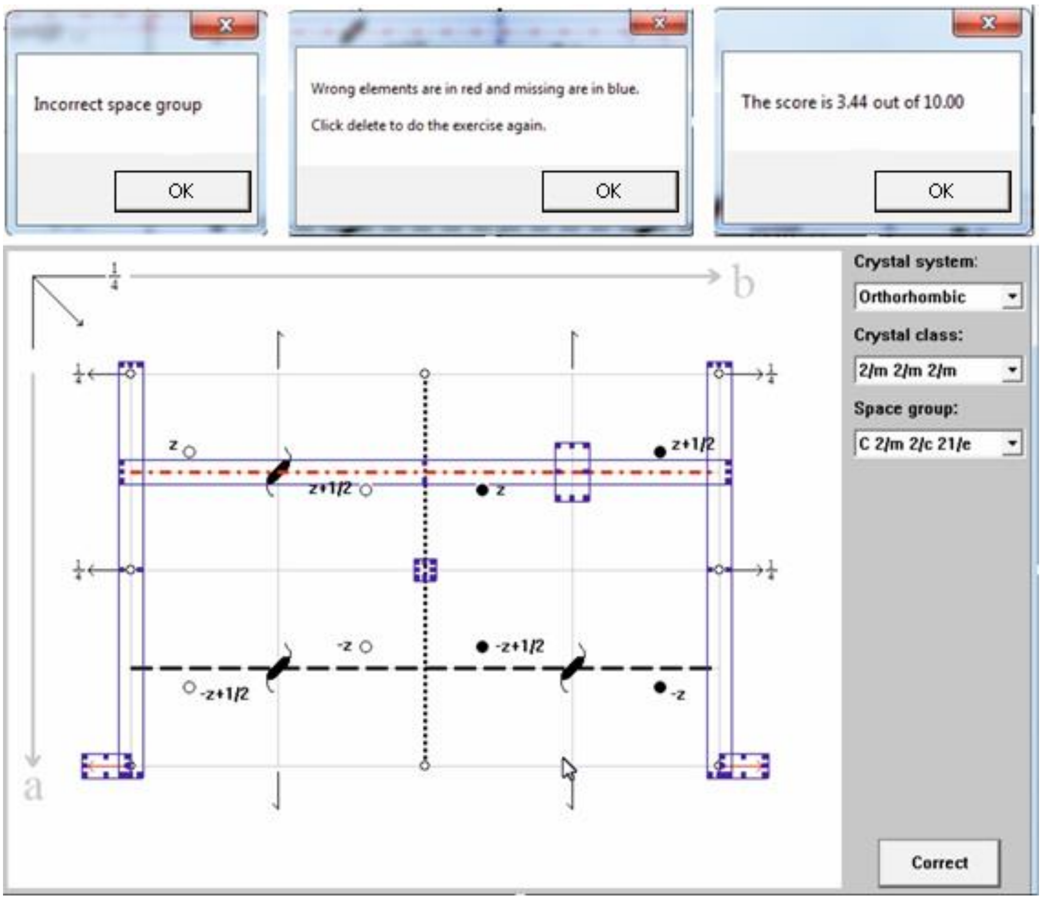

Figure 3. Pop-up help windows that appear when the <Correct> button is clicked.

A quick user guide and an example of an SGS resolution can be found in the Supporting Information.

5. Software Design and Functionalities

The GESUS tool consists of two software components: the graphical user interface (GUI) and a folder with exercises files (Figure 4). The GUI was developed using the C++ programming language and is currently for Windows XP and higher versions. The exercises files are text files with a specific extension ".sgf" (space group file). These files include all the information about the symmetry of the space group but are encrypted so that such information is not directly accessible by the user.

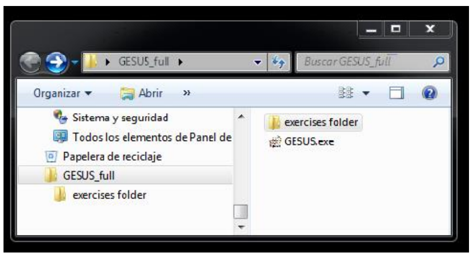

Figure 4. The two components of GESUS v. 2.4 are an executable file "GESUS.exe" that opens a graphical user interface (GUI) and an exercise folder.

It is a simple design application that does not require software installation, is easy to use with fast, successful learning, and only requires unzipping the executable file and library exercises. Currently, GESUS v.2.4 includes 74 space groups of symmetry for Triclinic, Monoclinic, and Orthorhombic.

The GESUS application currently allows two main types of exercises: drawing the symmetry elements of a space group from motifs/atoms distribution in the structure or drawing them from the name of the SGS.

GESUS is available for free download at: https://citius.us.es/gesus/index_en.html (accessed on 27 December 2021).

6. Impact and Student Impression

This application will have a positive impact on the teaching of space groups of symmetry for students of crystallography at a basic-medium level and for university students studying Chemistry, Physics, Geology, Science of Materials, etc., who have elementary knowledge about elements of symmetry, Bravais lattices, crystal classes, and wallpaper groups.

We have seen an evident improvement, in learning the subject of crystallography for chemists at the University of Seville, in students' grades after using this application, which demonstrates that the program helps students achieve a better conceptual understanding of how operators of symmetry work.

This section includes students' impressions using GESUS. The survey was carried out after the first evaluation exam of Crystallography, Chemistry Degree (University of Seville, June 2021). A total of 55 responses to an anonymous survey were obtained from these students. The survey results show the importance of GESUS as a self-learning/evaluation assistance for resolving SGS problems.

Of the students surveyed, 54 out of 55 (98.2%) were aware of GESUS; 5 students (9.3%) responded that they had not used GESUS; 31 of them had used GESUS more than 10 times (57.4%); and 6 students (11.1%) had used it only a few times (less than 3 times).

Students who responded that they had used GESUS at least once were asked about their satisfaction, and 59.2% gave the highest score (5 on a scale of 1 to 5) for the usefulness of GESUS for learning or consolidating knowledge to solve SGS exercises, 24.5% gave a rating of 4, and 14.3% a rating of 3. There was one response (2%) that gave a rating of 1 (minimum rating) (Figure 5, bar: "Utility"). Most of these students would strongly recommend the use of GESUS to other students (value of 5 for 67.3% and 4 for 20.4%), while six students would give a low recommendation (Figure 5, bar: "Recommendable").

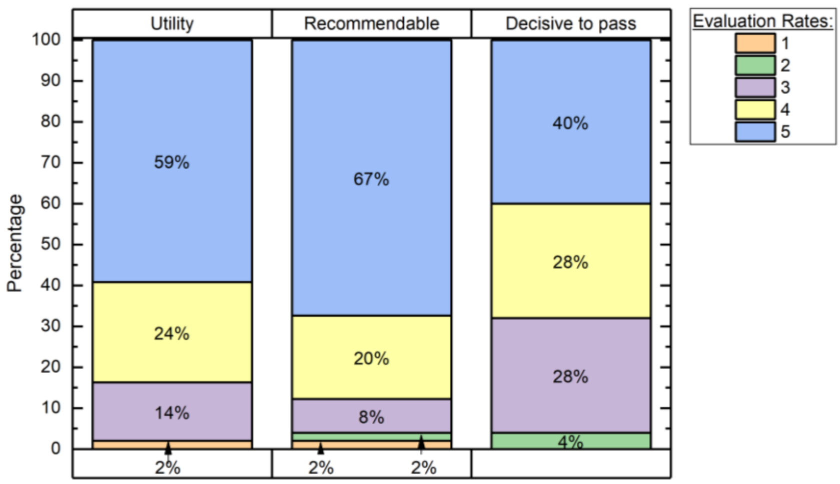

Figure 5. Statistical values of student responses related to the *utility* of GESUS for SGS learning, level of *recommendation* to other students, and how the use of GESUS had *influenced their ability to pass* the subject. Survey evaluation rates are 1 to 5.

Finally, the students who successfully passed the exam (51% of the students surveyed) rated positively (68% with levels 5 and 4) the influence of GESUS to pass the exam (Figure 5, bar: "Decisive to pass"), despite the fact that solving SGS exercises are only a portion of the subject's content. Although only half of the students passed the subject at the first evaluation exam round, this was significantly better than the average number of passes at the first exam round in the previous five years, around 35%. Of the students surveyed who passed the subject evaluation, 61.3% reported using GESUS on more than 10 occasions.

The survey was used as an opportunity to ask for suggestions for future improvements. They highlight, as suggestions, the possibility of displaying the Wyckoff positions and the cross-platform deployment of GESUS. Both suggestions are under development for an upcoming version.

This type of learning software is widely used since educational institutions promote the use of software for knowledge acquisition outside the traditional classroom and online.

To date, the program has been downloaded from a small number of places in Spain (from the IP downloads of the server). However, due to the impact of this publication and the addition of an English language option, a strong increase in international downloads is expected.

7. Conclusions

The GESUS application is used to learn how elements of symmetry act in the context of space groups.

The application self-evaluates and assesses the knowledge acquired, allowing the user to repeat each exercise until it is completed correctly with the appropriate recommendations.

Currently, this kind of interactive educational tool for gaming is in demand due to the benefits provided to students. The interactive multimedia software GESUS becomes a problem-solving tool, a conceptualizer, and a tutorial for the student.

Students in the crystallography subject of the Chemistry Degree, who were surveyed in July 2021, responded that GESUS showed satisfactory utility, is recommendable to other students, and facilitated their study and understanding of the SGS exercises. They considered GESUS to be highly influential in helping them to pass the subject.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/educsci12020085/s1. Document containing a quick user guide and an example of an SGS resolution.

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