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Visualizing and teaching crystallographic symmetry using *Jmol*

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The *Jmol* **Space Group Symmetry Visualizer** website provides a modular set of interactive pages for the visualization of symmetry groups, including both space groups and plane groups, as well as subperiodic groups (frieze, rod, and layer). Groups and group–subgroup relationships are illustrated using a variety of molecular and ionic structures.

1. Introduction

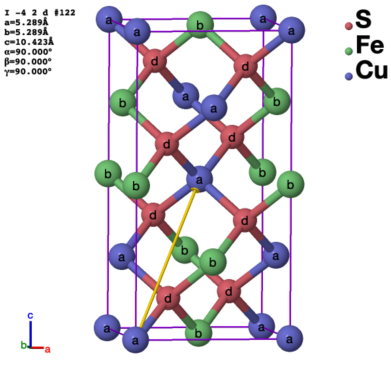
The *Jmol* **Space Group Symmetry Visualizer** (https://spacegroups.symotter.org) is an online resource for the visualization of crystallographic symmetry built around the versatile *Jmol* application. This website provides a modular set of interactive pages for the visualization of symmetry groups, including both space groups and plane groups, as well as subperiodic groups (frieze, rod, and layer). Groups and group–subgroup relationships are illustrated using a variety of molecular and ionic structures. All symmetry elements are color-coded and can be selectively displayed for easy comparison to conventional space group diagrams. Wyckoff positions are presented in tabular form, and representations can be generated and interactively dragged, maintaining their respective symmetry relationships. Atoms in structures are listed by Wyckoff position and can be labeled and colored by element, Wyckoff, or site symmetry. Maximal subgroups for all space groups are listed, and representations of group–subgroup relationships are easily generated. Taken together, these capabilities represent a unique resource for students and educators in crystallography and researchers using crystallographic methods.

2. Resources for teaching crystallographic symmetry

The challenge of teaching crystallographic symmetry is evident considering the numerous resources that have been created and the variety of approaches described in the literature (Enemark, 1988; Cooper *et al.*, 1989; Hardgrove, 1997; Boo & Mattern, 2008; Pett, 2010; Chapuis, 2011; Gražulis *et al.*, 2015; Ruiz & Johnstone, 2020; Dong & Zheng, 2021; Zheng & Campbell, 2021; Kotsis, 2025).

2.1. Two-dimensional symmetry diagrams and tutorials

Teaching crystallographic symmetry requires the communication of three-dimensional concepts using primarily two-dimensional representations. A common approach is to use the two-dimensional plane groups to introduce symmetry concepts and terminology that can later be extended to space groups (Brady, 1978; Stróż, 2003; Duda *et al.*, 2020). Plentiful



examples from textiles and the decorative arts (Glasser, 1967; Hargittai & Lengyel, 1984; Hargittai & Lengyel, 1985; Schoeni *et al.*, 2013) provide an accessible and engaging approach for students at all levels. The advent of personal computers allowed the creation of programs to display space group diagrams and molecular representations (Penfold & Temple, 1982; Temple, 1985). As computers became more capable, software like Margaret Kastner's pioneering *Crystallographic Courseware* (Kastner, 1999; Kastner *et al.*, 2000; Kastner *et al.*, 2013) provided instructional material covering many topics, including symmetry, asymmetric units, plane groups, and reading the International Tables for Crystallography (Aroyo, 2016). In a similar vein, the excellent *Symmetry and Space Group Tutorial* developed by Bruce Foxman and Jerry Jasinski (Foxman, 2021) utilizes careful step-wise building up of space group diagrams and occasional humor to create an effective and enjoyable tutorial. The recently developed GESUS (Grupos Espaciales de Simetria de la Universidad de Sevilla) application provides an interactive environment where students can learn symmetry operations and conventional representations through a set of tutorial exercises (Miras *et al.*, 2022).

2.2. Three-dimensional physical models

The use of physical models has a long history in crystallography and structure determination, so it is not surprising that models, ranging from ball-and-stick to papercraft to 3D-printed objects, have been employed for teaching space groups, Bravais lattices, and crystal forms (Hathaway, 1979; Sein & Sein, 2015; Graw & Stalke, 2022; Aristov *et al.*, 2022). The opportunity for students to build or physically interact with models can lead to insights and understanding about how molecules are arranged in unit cells and their symmetry relationships. Creative use of inexpensive materials makes these models accessible for a wide range of audiences.

2.3. Three-dimensional computer representations

With the advent of high-quality color computer graphics displays, the power and potential to display three-dimensional crystal structures and space group symmetry was realized by several groups (Abad-Zapatero & O'Donnell, 1987; Sakurai *et al.*, 1989) and eventually became part of commercial software packages (Khosrovani *et al.*, 1999). As personal computers have become more powerful, increasingly complex images and videos have been produced (De Graef, 1998; De Graef, 2009; Bucio *et al.*, 2024) to support the teaching of crystallographic symmetry. Other educators have embedded three-dimensional figures of the 32 crystallographic point groups into PDF files (Arribas *et al.*, 2014) and created animations and videos for teaching space group symmetry (Bucio *et al.*, 2024). Hitzer and Perwass have created the *Space Group Visualizer* (Hitzer & Perwass, 2006; Hitzer & Perwass, 2021; Hitzer *et al.*, 2010; Müller, 2021), a stand-alone computer program (Windows) for the three-dimensional visualization of space groups and their associated symmetry operations. More recently, computer models in virtual reality environments have been used to introduce space group symmetry, including the overlay of symmetry element representations on crystal structures (Graw *et al.*, 2022; Graw *et al.*, 2023; Mercado, 2025).

2.4. Molecular visualization software

Numerous molecular and crystal structure viewing programs developed over the years include the capability to display crystallographic symmetry information (de la Flor *et al.*, 2024). Some examples include *MAGE* (Pavkovic, 2005), *Diamond* (Wu, 2024), *VESTA* (Momma & Izumi, 2011), *Mercury* (Macrae *et al.*, 2020; Battle *et al.*, 2010), and *Jmol* (Hanson, 2010*a*; Hanson, 2010*b*; Hanson, 2017). Within this set of programs, *Jmol* occupies a unique position due to its extensive capabilities, flexibility, and scripting language. Originally developed as an open-source molecular viewing program written in Java, work by Howard starting in 2002 added browser applet capability that allowed integration of the *Jmol* applet into web pages (Howard *et al.*, 2010). Significant revisions and continued work by Hanson has added extensive crystallographic capabilities to *Jmol*, including reading of crystallographic (CIF) data files, display of unit cells and symmetry elements, and comprehensive space group information, all in a well-documented scriptable environment (de la Flor *et al.*, 2024; Hanson, 2025*a*; Hanson, 2025*b*). *Jmol* is also unique in that the same codebase produces both the stand-alone Java program (Jmol.jar) and a JavaScript-based web application (sometimes referred to as *JSmol*, but herein referred to simply as *Jmol*) that can be embedded into any web page.

In this article, we will focus on the development and implementation of a browser-based space group symmetry visualizer, demonstrating how *Jmol* can serve as the foundation for a dynamic, interactive, and effective tool for visualizing and teaching crystallographic symmetry.

3. Design principles

When designing and implementing a website for teaching and sharing molecular and crystallographic symmetry, our efforts focused on making materials that are accessible, intuitive, and modular. The features of *Jmol* make it possible to create materials that meet all of these goals.

By considering accessibility, we seek to lower the barriers to use by students and implementation by instructors. Accessibility in this context refers to electronic materials that have no requirements beyond a web browser. The visualizations and controls are designed to be effective on a range of devices from laptops to mobile devices and run independent of any other software or applications. Additionally, web pages are designed to be *responsive*, adapting to screen size and orientation. Download sizes for web pages are minimized, taking advantage of the modular structure of *Jmol*, which loads required components dynamically as needed.

Intuitive design, while more subjective, focuses on creating a resource where most actions can be completed by selecting options from a menu, list, or checkbox. The layout follows that

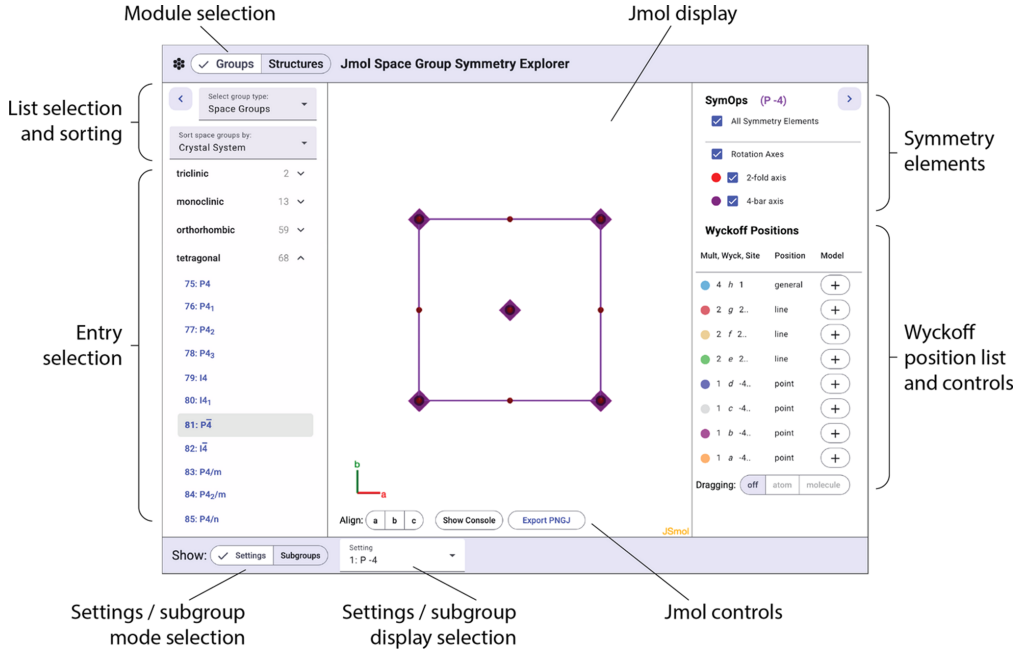


Figure 1
An annotated view of the *Jmol* **Space Group Symmetry Visualizer** page displaying the $P\bar{4}$ space group and its respective symmetry elements and Wyckoff positions.

of common websites and apps using conventional elements for buttons and other controls. The interface is relatively simple, with the majority of the screen dedicated to the *Jmol*-based interactive display of space group and molecular representations. All representations are color-coded with legends that clearly indicate all aspects of the diagrams. Google's Material Design (Google, 2025) is used throughout to provide an accessible and familiar interface.

The modular aspect of these materials makes the site adaptable to a wide range of objectives. This design choice allows the various modules to be tailored for audiences at different levels. There is no pre-determined path or order in which to use the materials, so students and instructors are free to adapt them to their individual needs and environments. The menu-driven selections and interactive click-and-drag visualizations are intuitive and accessible, thereby appropriate even

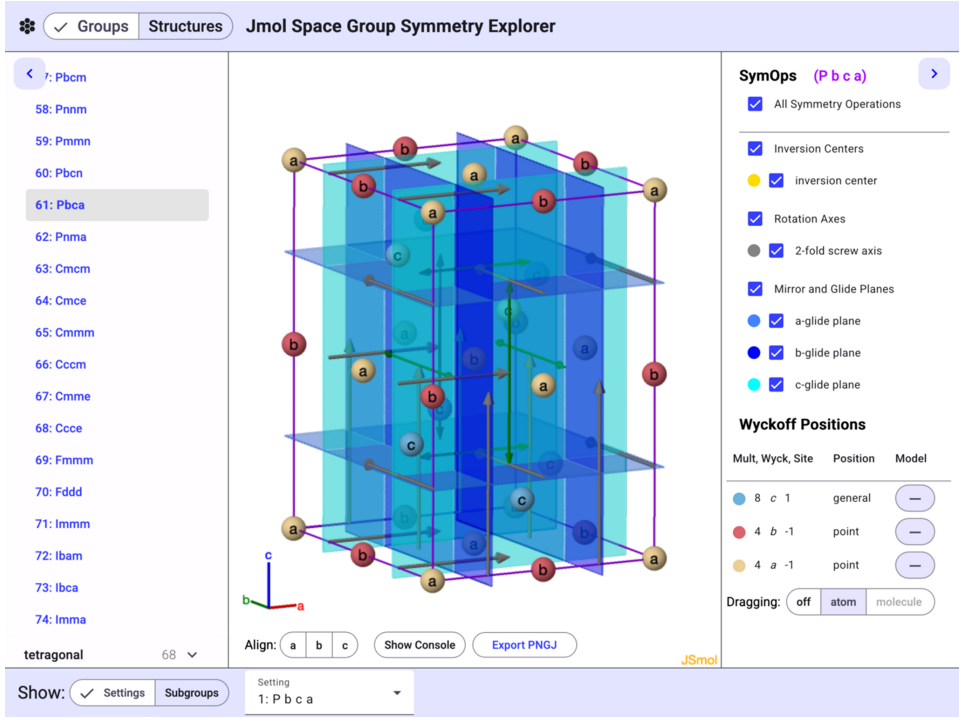


Figure 2
An illustration of the symmetry elements and Wyckoff positions of the *Pbca* space group.

at an introductory level. For those students and instructors who wish to explore beyond what is exposed by the interface, the *Jmol* scripting environment is always available from a pop-up scripting console. Additionally, users can construct representations and share them as a 'pngj' file, a standard PNG image format that also contains the full *Jmol* state, allowing the image to be drag-dropped into the *Jmol* Java application or other web pages that utilize *Jmol*.

4. Website overview

The site is organized into two modules: (1) the symmetry group visualizer, and (2) the crystal structure symmetry visualizer. A large toggle button at the top of the page switches between the two modules.

4.1. Symmetry group visualizer

The symmetry group visualizer is arranged into three panels, as shown in Fig. 1. On the left are controls for selecting and sorting the group list along with the list itself. Available symmetry groups include space, plane, frieze, rod, and layer groups. Lists can be sorted by system, class, or number. Selecting a symmetry group displays a three-dimensional representation of the group in the center panel that at first glance appears to be simply a colorized version of the standard plane-group representations appearing in textbooks and tables of space groups. But clicking and dragging in the center panel rotates the representation. The right panel displays a list of symmetry elements and a table of Wyckoff positions. The display of symmetry elements can be toggled on and off using the respective checkboxes. The Wyckoff table includes buttons that allow the user to add and delete pseudoatoms representing the respective Wyckoff positions in the unit cell. Toggling the **dragging** option at the bottom of the list to **atom** allows these atoms to be dragged in three-dimensional space. All the symmetry-related atom positions will update dynamically. Atoms in special positions can only be dragged within the constraints defining their Wyckoff position – a plane, axis, or fixed point. Attempts to drag any atom – special or general – to a different Wyckoff position will not be successful, and a graphical warning symbol will be generated.

A more detailed example of the visualizations made possible by *Jmol* is shown in the *Pbca* space group example found in Fig. 2. The inversion centers, twofold screw axes, and glide planes are all illustrated in the three-dimensional representation with controls and a color-coded key shown on the right side. *Jmol* differs from other programs such as *Mercury* in that it uses unique colors for each of the different types of glide planes and different colors for screw axes of opposite handedness as well as n-bar axes. Representations of all the Wyckoff positions have been added and are shown as colored spheres with labels.

4.1.1. Space group settings

By default, the symmetry group visualizer will show the standard setting for a space group, but all the available settings for the selected group are available in a drop-down selection box at the bottom of the page. The display and list of symmetry elements will update as needed when a different setting is

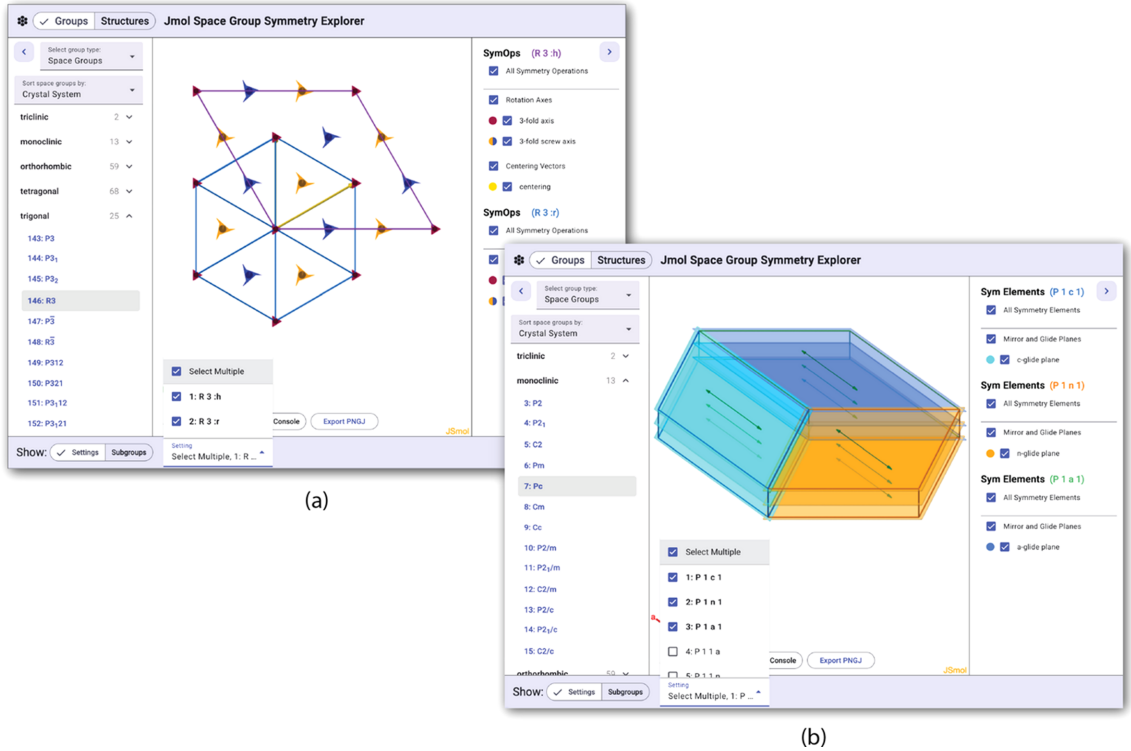


Figure 3
Examples of the display of multiple settings for two different space groups: (*a*) the hexagonal and rhombohedral settings of the *R*3 space group, and (*b*) the *Pc* setting along with the equivalent but non-standard *Pn* and *Pa* settings.

selected. There is also the option in the drop-down menu to select and overlay representations of multiple settings. Two illustrative examples displaying multiple settings for the *R*3 and *Pc* space groups are shown in Fig. 3.

The symmetry elements for all settings are listed in the panel on the right-hand side. This allows direct comparison, showing, for example, that there is no centering vector in the rhombohedral setting of *R*3 and the *c*-, *n*-, and *a*-glide planes in the *Pc*, *Pn*, and *Pa* settings are all equivalent.

4.1.2. Plane and other groups

All of the features described above are also available for any of the plane, frieze, rod, and layer groups. These simpler representations can be particularly useful in an educational context as stepping stones to the more complex space groups. An illustration of the *p*2*mg* plane group is shown in Fig. 4 with spheres representing the available Wyckoff positions.

Another representation that is potentially valuable for educators is illustrated in Fig. 5, showing the rod group $p6_1$ and a representation of the corresponding general position. The 6_1 screw axis is clearly shown and the pseudoatoms can be dragged, with all other symmetry-equivalent positions updating to reflect the underlying symmetry. Other symmetry relationships can be readily illustrated using similar plane, rod, and layer groups.

4.1.3. Maximal subgroups

Jmol is also capable of generating lists of space group–subgroup relationships and displaying informative representations of the resulting symmetry relationships. Switching the toggle bar at the bottom left of the website to subgroups will display a list of the maximal subgroups of the currently selected group. Selecting one of the subgroups will generate an overlay of the two groups, with pseudoatoms at general positions representing the symmetry of the original group and colored according to their symmetry in the subgroup. An example group–subgroup relationship, 99 > *a*–*b*,*a*+*b*,*c* > 35 in CLEG notation (Hanson, 2025*a*), is shown in Fig. 6.

4.2. Structure symmetry visualizer

The layout of the structure symmetry visualizer (see Fig. 7), selected using the toggle bar at the top left, is similar to the group visualizer. On the left is the list of structures, the *Jmol* display is in the center, and information and controls are on the right. Two sources of structural data are available. The first option is the AFLOW library of crystallographic prototypes (Mehl *et al.*, 2017). This set includes the option to filter the list by number of unique elements, making it possible to limit the list to elemental crystal structures or binary salts, for example. The second set comprises a curated set of representative structures taken from the Cambridge Structural Database (CSD; Groom *et al.*, 2016). Entries were selected by searching for representative structures from each space group and prioritizing structures with a minimal number of atoms in the asymmetric unit.

Symmetry elements, off by default, can be selectively displayed using the checkbox controls in the right panel. Additional information includes a list of atoms in the asymmetric unit, along with their respective Wyckoff positions. The packing controls fill the unit cell, the unit cell extended by

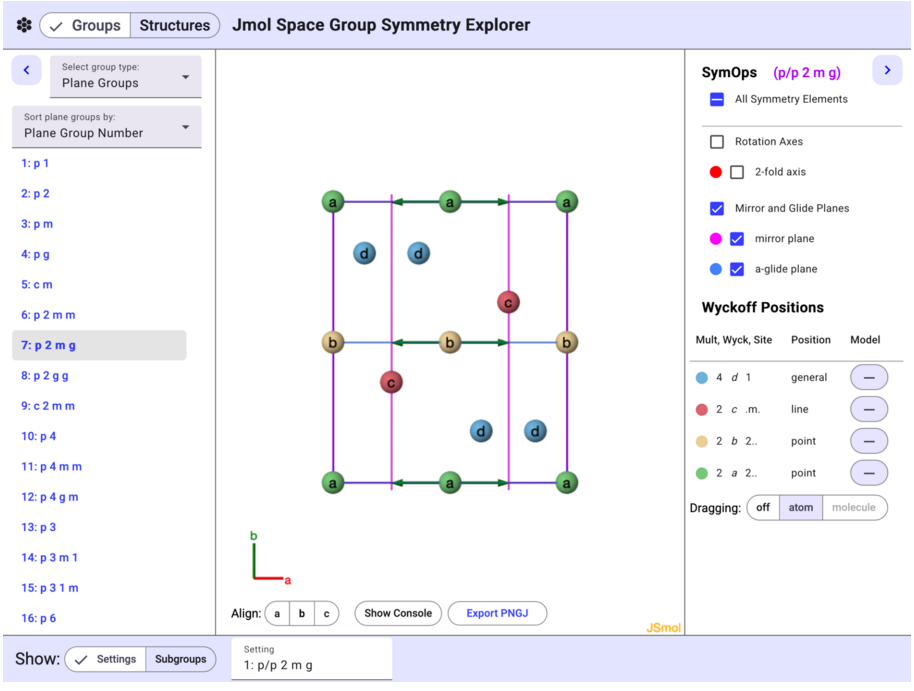


Figure 4
The *p*2*mg* plane group showing mirror planes, glide planes, and Wyckoff positions. Note: twofold axes are omitted so as to not obscure the Wyckoff labels.

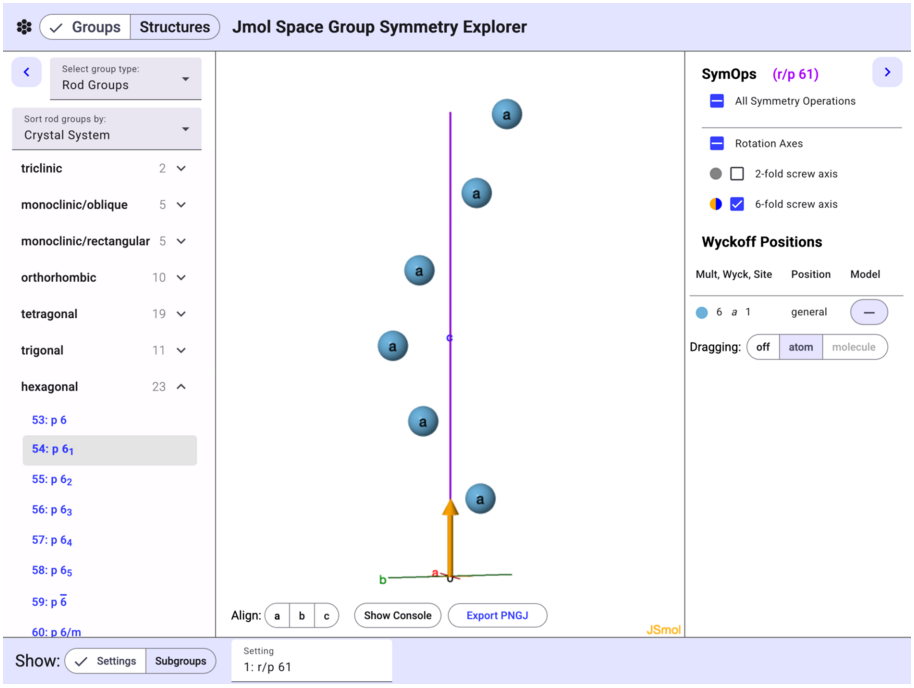


Figure 5
The $p6_1$ rod group with a set of atoms representing general positions. Note that the rod group is periodic only in the c direction. The 3D coordinates of the atoms are constrained by the sixfold screw axis.

closest neighbors, or with molecules within the unit cell. Atoms can be colored and/or labeled by element, by Wyckoff position, or by site symmetry. Depending on the type and symmetry of the structure, molecules or atoms of the structure can be dragged and the position of symmetry-related molecules or atoms will be updated in real time. Information about the structure and links to the respective database are shown in the bottom toolbar.

An example molecular structure, diiodomethane, entry DIMETH02 in the CSD (Prystupa *et al.*, 1989), is illustrated in Fig. 8. The space group is *Fmm*2, with the C, H, and I atoms each occupying a unique Wyckoff position. The mirror and

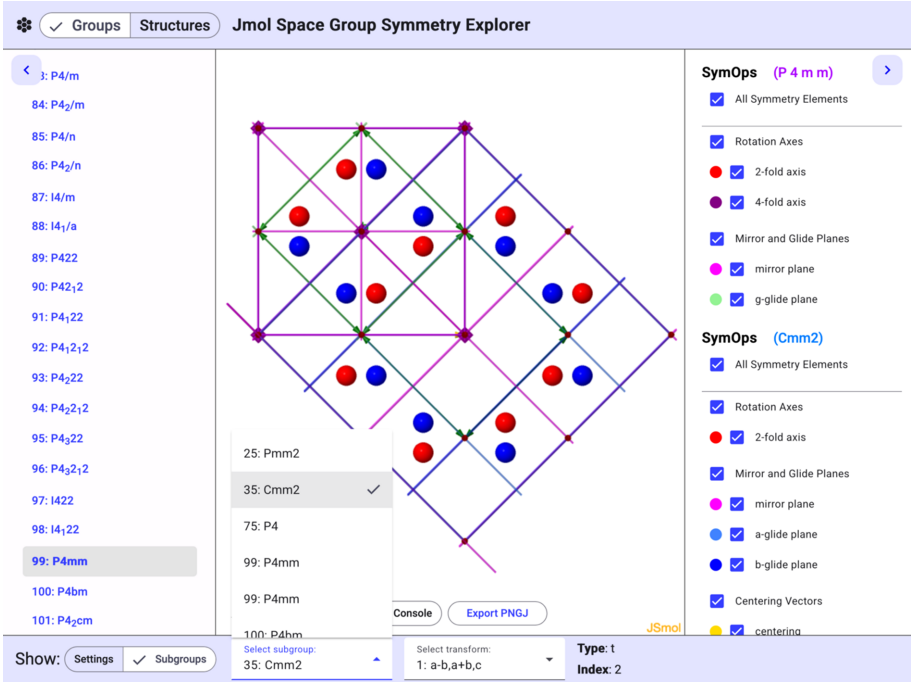


Figure 6
The *P4mm* to *Cmm*2 (99 > *a*–*b*,*a*+*b*,*c* > 35) group–subgroup transformation.

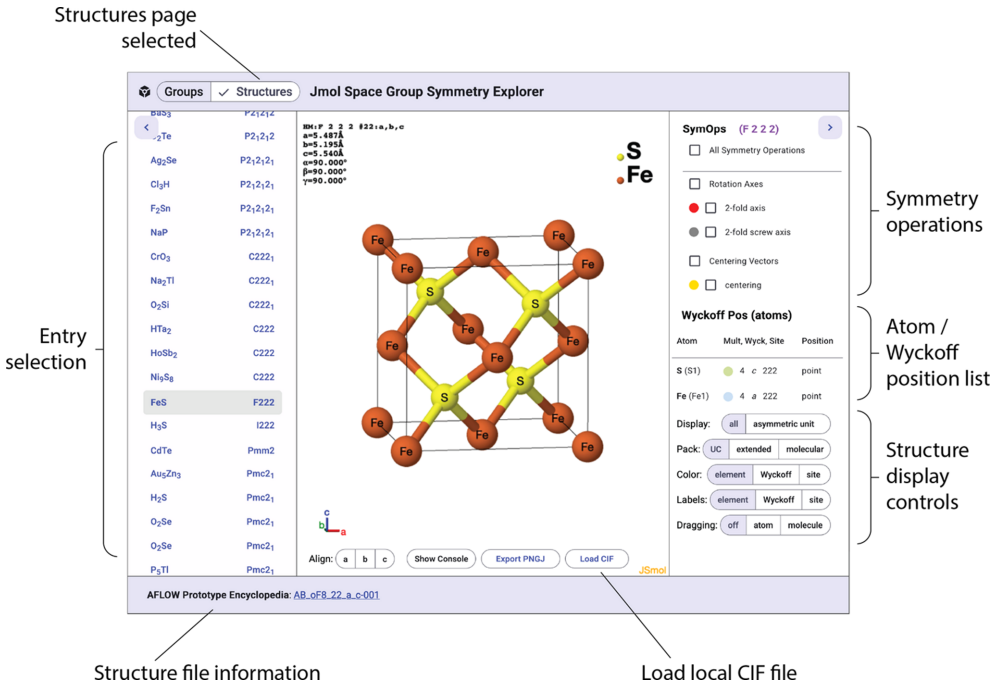


Figure 7
An annotated view of the *Jmol* **Structure Symmetry Visualizer** displaying the structure of FeS (space group *F*222).

glide planes are all clearly identifiable using the legend in the right panel. The C atoms are located on the twofold rotation axes at the intersections of the perpendicular mirror planes, corresponding to Wyckoff position *a*.

The option to color atoms by Wyckoff position is highlighted in Fig. 9 with the structures of (*a*) $FeCuS_2$ and (*b*) hexamethylenetetramine.

4.2.1. Reading local CIF files

The existing website includes nearly 2000 example structures, but it can also load and display structures from local CIF files. The 'Load CIF' button at the bottom of the *Jmol* display provides a prompt from which the user can select a local file. The file will be loaded into the site, the structure displayed,

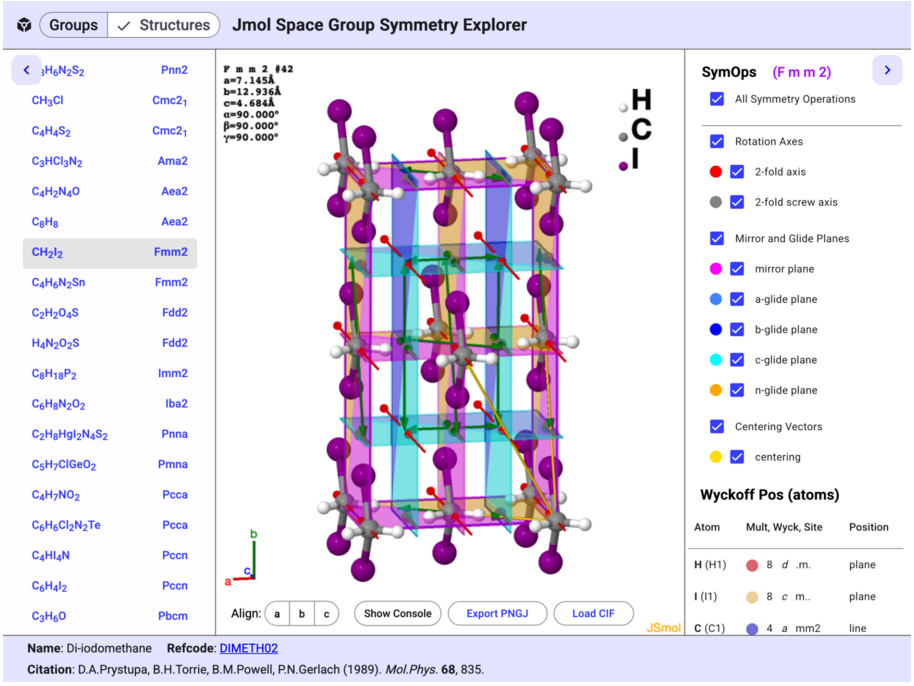


Figure 8
The unit cell of diiodomethane (space group *Fmm*2, CSD entry DIMETH02), illustrating the rotation axes, mirror and glide planes, and centering vectors.

and the symmetry elements and atom list with Wyckoff information will be shown in the right panel. Alternatively, users can just drag and drop a CIF file onto the *Jmol* display of the web page and the structure will load and display the relevant information and controls.

4.3. Additional export and sharing features

4.3.1. PNG file export

Jmol has the capability to generate a special form of png (portable network graphic) file that is both a capture of the current display *and* the full *Jmol* state. When these files are opened or dropped onto a *Jmol* instance in a web page or opened with the stand-alone Java *Jmol* program everything in the current structure/representation will be regenerated.

4.3.2. URL sharing

The website is designed to provide identifying information for the current model or structure in the browser address bar so users can share a particular space group or structure by simply copying the current URL.

5. Examples and tutorials

A set of examples and tutorials has been created and is available as part of the supporting information associated with this article. These materials include:

– Step-by-step interactive tutorials covering inversion, reflection, rotation, rotoinversion, screw, and glide operations. Selected rod groups are used to focus on a single operation/element in each case. Interactive dragging of pseudoatoms helps reinforce the symmetry relationships between sets of atoms.

– Annotated examples of plane groups and space groups, building on the representations introduced in the earlier tutorial. The addition of two- and three-dimensional motifs help emphasize the transformations resulting from glide and screw operations.

– Three examples illustrating Wyckoff positions and their site symmetries. The tutorials include examples of pseudoatoms that are positionally constrained to a plane, line, or point, emphasizing the connection to the site description in the corresponding table.

– Two structural examples, one molecular, one ionic, illustrating Wyckoff positions and the asymmetric unit.

– Three examples illustrating space group–subgroup relationships.

We hope that these examples serve to illustrate just a few of the ways that this website can be used to inform and inspire students to learn and practice crystallography.

6. Conclusions

The *Jmol* **Space Group Symmetry Visualizer** website combines the crystallographic capabilities of *Jmol* with a web interface to create a flexible resource for the visualization of symmetry in crystallography. These materials provide a modular set of accessible and intuitive resources for students and faculty interested in the teaching and learning of crystallography and crystallographic symmetry.

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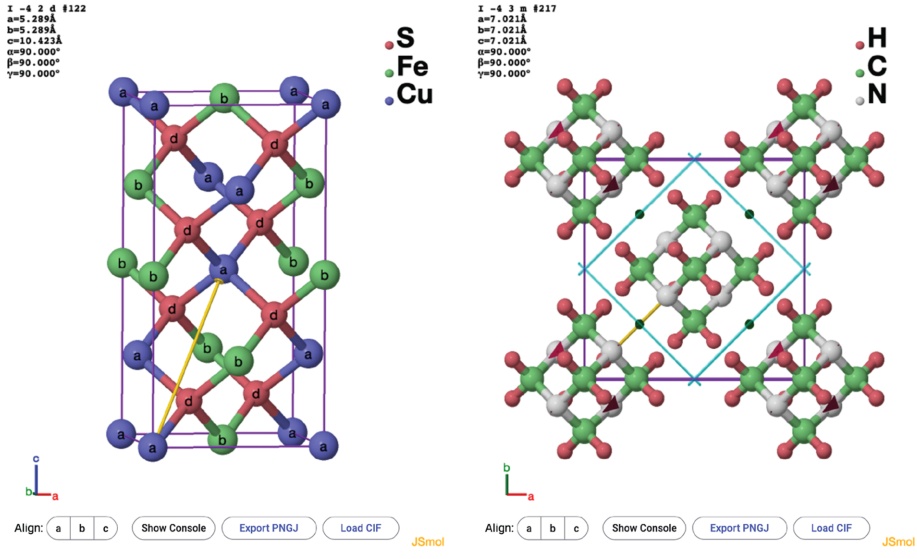

Figure 9
Two different structures, (*a*) $FeCuS_2$ (space group $I\bar{4}2d$) and (*b*) hexamethylenetetramine (space group $I\bar{4}3m$), each with the atoms colored and labeled by Wyckoff position.

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