TUTORIAL ON THE VISUALIZATION OF SYMMETRY-ADAPTED MODES AS DETERMINED WITH AMPLIMODES (BILBAO CRYSTALLOGRAPHIC SERVER)

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This is a tutorial on some methods for visualizing the distortion symmetry modes of any distorted structure, if determined using the program AMPLIMODES of the Bilbao Crystallographic Server. This tutorial shows how the output of AMPLIMODES can be combined with various programs, such as STRCONVERT, VESTA, Jmol and also FullProf to produce images, both static and dynamic, of the distortion modes determined by AMPLIMODES.

1. Introduction

The use of symmetry-adapted modes in the description of distorted structures is a powerful methodology that introduces a natural physical hierarchy among the degrees of freedom of the structure. This is not only useful in the analyis of the possible physical mechanisms underlying the stabilization of the system, but it can also be of utter importance in the crystallographic investigation of the structure, as the weigth of the structural parameters introduced in a symmetry mode description is in general hierarchized. Since the theoretical background is usually complicated with the heavy involvement of the theory of irreducible representations, people have, until recently, not made much use of this powerful analysis method, but thanks to computer implementations such as the program AMPLIMODES[1,2], which can be found in the Bilbao Crystallographic Server (http://www.cryst.ehu.es/cryst/amplimodes.html) [3, 4, 5] and ISODISTORT[6] (http://stokes.byu.edu/iso/isodistort.php) within the ISOTROPY Suite, this situation has drastically changed. Nowadays, applying these computer tools, symmetry mode analysis of distorted structures can be systematically and rapidly done and they require a minimal basic knowledge of the underlying group theory. Detailed information on these tools can be found in their respective references. Also a very through, step-by-step tutorial for AMPLIMODES is available in the webpage of the program. We will assume that the reader has some basic knowledge of this latter program, based on the mentioned tutorial and/or on the mentioned references. We will take the output of AMPLIMODES for a particular case study, and we will review the possible most direct visualization methods of the symmetry-adapted distortion modes described in this ouput. Apart from AMPLIMODES itself, various software such as VESTA [7], Jmol [8], STRCONVERT [9] and/or FullProf [10] can be employed in the visualization process.

2. Use of AMPLIMODES

Let us consider the orthorhombic phase of $SrZrO_3$ with space group *Pnma* (N. 62). This structure is a distorted perovskite, i.e. the structure derives from an ideal cubic structure with space group *Pm-3m* (N. 221) via a structural displacive distortion. The essential data defining these two structures are presented in Tables 1 and 2.

Table 1: Parent high-symmetry structure of $SrZrO_3$. This parent high–symmetry estructure does not need to be an experimental one. A virtual high-symmetry (reference) structure with the orthorhombic distortion deleted can be obtained from the experimental structure using PSEUDO.

```
# Space Group ITA number
221
# Lattice parameters
4.084 4.084 4.084 90 90 90
# Number of independent atoms in the asymmetric unit
3
# [atom type] [number] [WP] [x] [y] [z]
Sr 1 1a 0.0 0.0 0.0
Zr 1 1b 0.5 0.5 0.5
O  1 3c 0.5 0.0 0.5
```

Table 2: Structure of $SrZrO_3$ in its phase of *Pnma* symmetry (icsd database 184465). The structure has been transformed to a *Pnma* standard setting from the *Pbnm* description used in the original database entry.

```
# Space Group ITA number
62
# Lattice parameters
5.8206 8.1949 5.8045 90 90 90
# Number of independent atoms in the asymmetric unit
4
# [atom type] [number] [WP] [x] [y] [z]
Sr 1 4c 0.524000 0.250000 0.004000
Zr 1 4a 0.000000 0.000000 0.000000
O 1 4c -0.013000 0.250000 -0.069000
O 2 8d 0.284000 0.036000 0.215000
```

The *Pnma* standard setting of the orthorhombic structure can be related with the unit cell of the parent cubic structure through the basis transformation (a+b, 2c, a-b; ½, ½ , ½), where the second part of the transformation indicates the shift of the origin. It is important to note that this origin shift depends on the form chosen for the description of the parent structure (Sr at the origin).

We enter in AMPLIMODES the two structures described above as high and low-symmetry structures, either in the format shown above or as cif files, together with the aforementioned transformation relating the settings of the structures. If this transformation is not known, we could have used the available link to STRUCTURE RELATIONS to obtain a possible one. After submission, AMPLIMODES provides a summary of the symetry-mode decomposition of the distortion present in the *Pnma* structure with respect to the reference parent structure of the input. This is shown in Figure 1.

Summary of Amplitudes

Warning: Amplitudes are given for modes normalized within the primitive unit cell of the distorted structure. Under this normalization, mode amplitudes in distorted structures with different multiplication of their primitive unit cell are not directly comparable.

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(1/2,1/2,1/2)	R4-	(0,a,-a)	Imma (74)	2	0.0523
(1/2,1/2,1/2)	R5-	(0,a,a)	Imma (74)	1	1.1517
(0,1/2,0)	X5-	(0,0,0,-a,0,0)	Cmcm (63)	2	0.3153
(1/2,1/2,0)	M2+	(a,0,0)	P4/mbm (127)	1	0.7970
(1/2,1/2,0)	M3+	(a,0,0)	P4/mbm (127)	1	0.0116

Global distortion: 1.4366 Å

Figure 1. Summary of symmetry-adapted distortion modes amplitudes as presented in AMPLIMODES. Notice that the irrep labels are in general not unique and depend on the choice of setting employed for the parent structure. If the alternative setting with the Zr atom at the origin were used, the irrep labels employed to describe the symmetry of the modes would be different.

In addition to this summary, the description of each of these distortion symmetry modes is available by clicking on "Detailed information". This information for the particular case of the R5- distortion mode present in the structure is shown in Figure 2.

Irrep: R5-

Direction: (0,a,a)

Isotropy Subgroup: 74 Imma D2h-28

Transformation matrix:

```
[     1     0     1 ] [      0]
[     1     0    -1 ] [      0]
[     0     2     0 ] [    1/2]
```

The amplitude of this distortion is:
A_{R5-}= 1.1517 Å

There is one mode with this symmetry, and its amplitude in Ångströms is:

O1 1
1.1517

Normalized polarization vector expressed as displacements (in cell relative units) of the atoms in the asymmetric unit of the structure:(normalization unit: 1 Ångström)

Atom	δx	δy	δz
Sr1	0.0000	0.0000	0.0000
Zr1	0.0000	0.0000	0.0000
O1	0.0000	0.0306	0.0000
O1_2	0.0000	0.0000	0.0612

Virtual structure with only this symmetry component of the distortion frozen.
Submit to STRCONVERT to visualize and export this mode's displacements

Figure 2. Detailed information on the R5- distortion mode in the *Pnma* $SrZrO_3$ structure, as obtained in AMPLIMODES

In general a distortion symmetry mode is a combination of several symmetry modes of the same symmetry (irrep), and AMPLIMODES provides the relative amplitudes of each of them within a normalized total mode (the so-called polarization vector of the mode). But in the present case, there is a single symmetry mode involved, and the listing shows only its total amplitude. Separately the atomic description of the global normalized mode (polarization vector) is also given, showing the displacements associated with each atomic site in the asymmetric unit (the atomic displacement corresponding to any other atom can then be obtained making use of the *Pnma* symmetry operations). From the table showing the atomic displacements describing the polarization vector of the distortion mode, one can easily see that this R5- distortion mode only involves some correlated displacements of the oxygen atoms, while the other atoms do not move.

In a more general case, as the one of the X5- distortion mode, two symmetry modes are involved (the number of symmetry modes composing the distortion mode is shown in the column "dimension" of the summary shown in Figure 1), and then the output also provides the amplitudes of the two symmetry modes in the polarization vector of the experimental X5- distortion mode.

As a final step, we save for later use the output of AMPLIMODES as a html file with the title: modes_SrZrO3.html.

In summary, using AMPLIMODES, for some given high and low symmetry structures, together with the transformation matrix relating their two unit cell bases, we can identify the symmetry distortion modes that are present in the low symmetry structure when compared with the given high-symmetry structure, and obtain their amplitudes. In the next section we will describe some ways to visualize these symmetry-adapted distortion modes. There are various ways and various software that can be used. We will start from the easiest method and move on from there to more complicated ones.

3. Visualizing the distortion symmetry modes with STRCONVERT AND VESTA

STRCONVERT was initially conceived to provide basic conversion between various structural data file types but soon many additional features were implemented as the need arose. In its current state, it is capable of interpreting and visualizing atomic displacements, meaning that we can use it for representing symmetry modes. Continuing with the R5- distortion mode of $SrZrO_3$ in the case study of the previous section (Figure 2), we can transport its associated atomic displacements to the STRCONVERT interface, as shown in Figure 3, when one clicks the button: "Submit to STRCONVERT to visualize and export this mode's displacements".

The atomic displacement values are transported taking into account the global amplitude of the distortion, hence the atomic displacements of the mode polarization vector are multiplied by the global mode amplitude (e.g., for O2, Δz = 1.1517 x 0.0612=0.0705, with 1.1517 being the amplitude of the distortion mode (Figure 1) and 0.0612 being the atomic displacement component in the normalized polarization vector of the mode, as given in Figure 2).

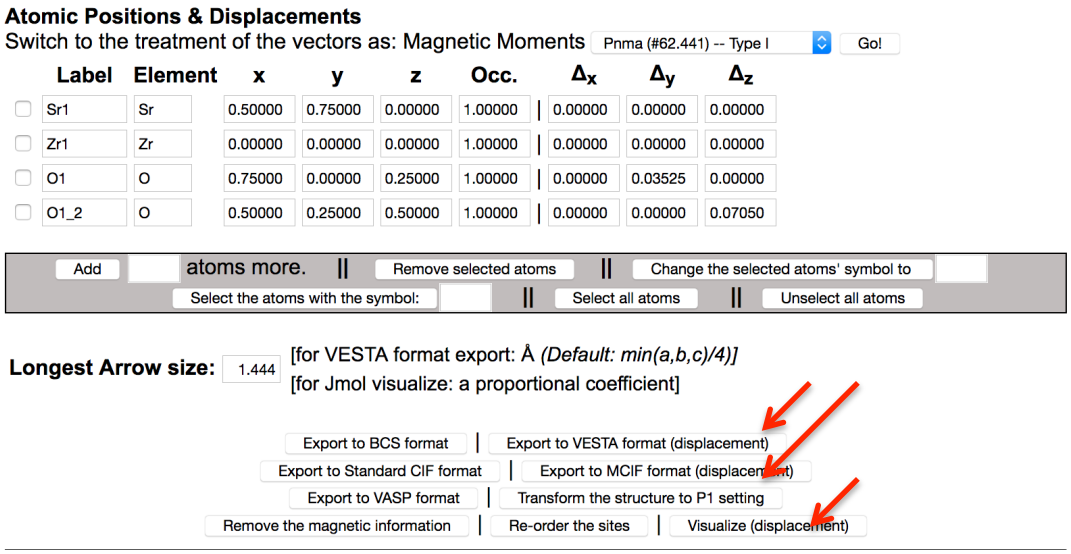


Figure 3. Information of the R5- mode as passed to STRCONVERT

From here on, we can proceed in various ways. The more robust and powerful one is to produce a file under the so-called magCIF format with the button "Export to MCIF format (displacement)" and then visualize this file (with extension .mcif), with the VESTA program. After clicking on the MCIF format button a link to download the corresponding file appears on the STRCONVERT menu webpage, as shown in Figure 4.

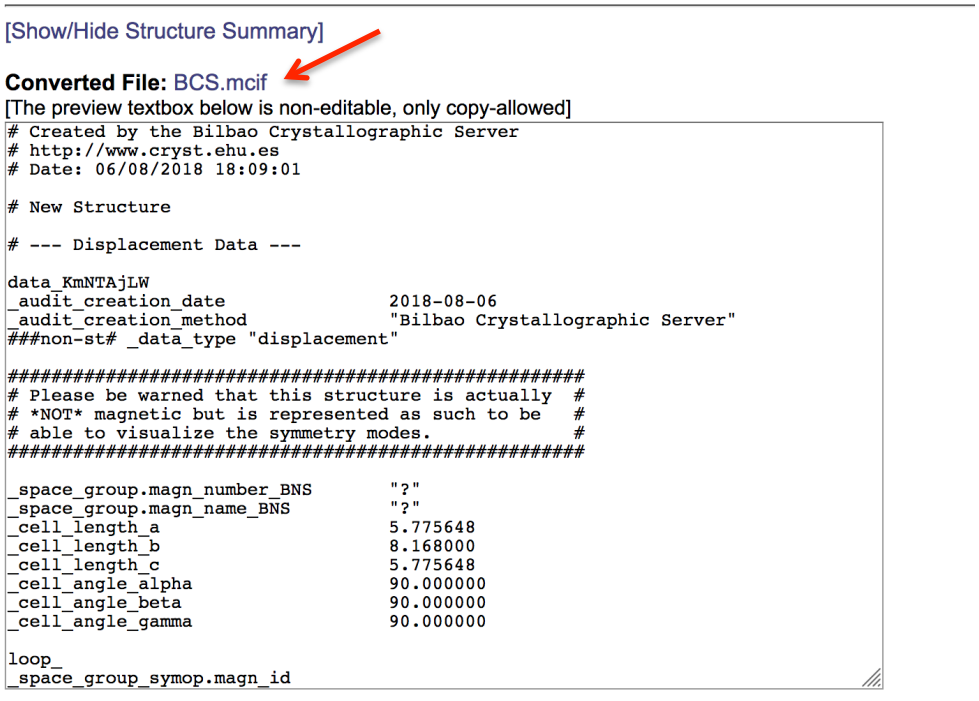


Figure 4. Partial screenshot of the interface webpage of STRCONVERT after clicking on the button "Export to MCIF format (displacement)", showing the file with extension .mcif that has been created. The file can be downloaded by clicking on "BCS.mcif".

The magCIF format is in principle intended for magnetic structures, and is directly readable by VESTA. The program uses it here as a trick to associate to each atomic site a vector representing the corresponding atomic displacement associated with

the mode, although in the file they would appear as magnetic moments. In other words, the file being produced describes a "fake" magnetic structure with the appropiate magnetic space group symmetry to reproduce correctly the relative values of the mode atomic displacements associated with any atom of the structure, when they handled by the program as magnetic moments under this magnetic space group. In this way, if this mcif file is loaded in VESTA, this program can visualize the correlated atomic displacements of the mode within any region of the structure, as vectors crossing the atoms (the traditional form that the magnetic moments are usually represented). As shown in Figure 4, the file contains a highlighted commentary warning about the real meaning of the file, the magnetic structure being only a trick to represent the mode using the feature of VESTA supporting magnetic structures described under the magCIF format.

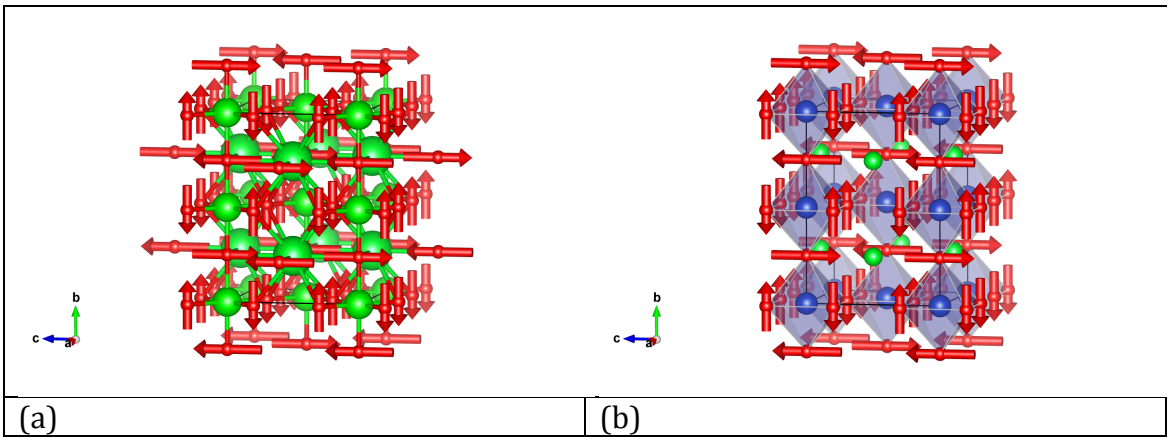


Figure 5. Visualization of the R5- mode done by VESTA after the loading of the corresponding .mcif file created by STRCONVERT. (a) direct visualization after loading; (b) the same after some editing of atom colours, bonding, and polyedral depiction.

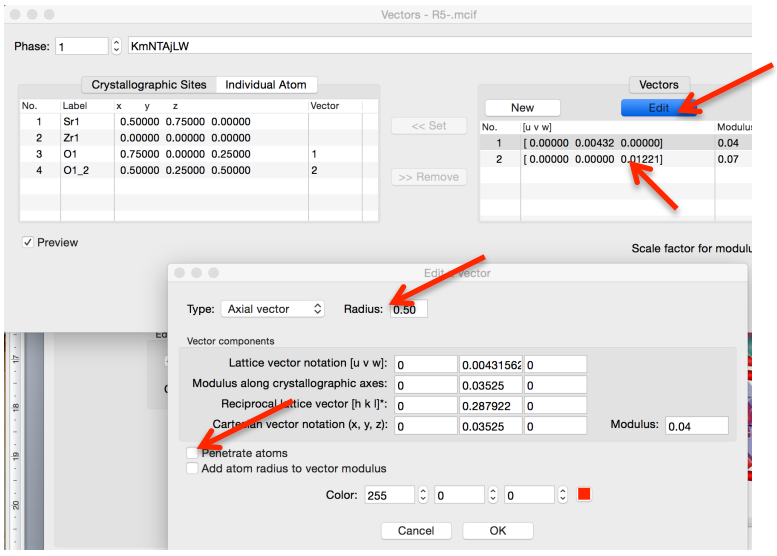


Figure 6. Screenshot showing the editing menu of vectors in VESTA, the main features to be considered in order to change the depiction of the atomic displacement vectors to its more usual form with the vector starting on the atom are indicated with red arrows. The option "Penetrate atoms" must be disabled.

Figure 5(a) shows the direct visualization of the R5- distortion mode done by VESTA after loading the .mcif file produced by STRCONVERT, while Figure 5(b) shows the result of some editing of atom colours, bonding, polyhedra depiction, etc. If we want now to represent the relative atomic displacements as arrows starting in the corresponding atom located at its reference high-symmetry, we have to use the corresponding editing menu of the vectors in VESTA, as shown in Figure 6. The option "Penetrate atoms" must be disabled for all listed vectors. The width of the arrow can also be changed by editing the value "Radius" of every vector, also shown in Figure 6. The final result is shown in Figure 7. It can be seen that this R5- distortion mode, which has the largest amplitude in the total distortion (see Figure 1), is essentially a "rigid-unit mode" of the ZrO_6 octahedra, i.e. the oxygens displace in such a way that the octahedra rotate and remain undistorted in a first approximation. The rotation axis is along the x direction in the *Pnma* setting.

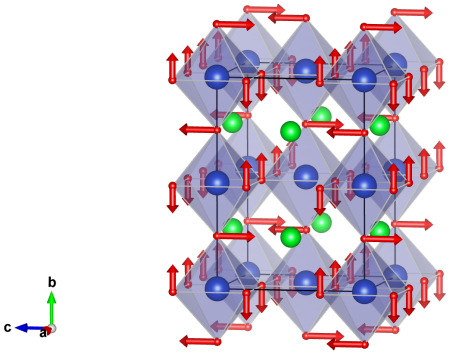


Figure 7. R5- distortion mode in the *Pnma* structure of $SrZrO_3$, as obtained with VESTA using the .mcif file created by STRCONVERT from the symmetry mode analysis of AMPLIMODES. This picture required some editing within VESTA, as explained in the text.

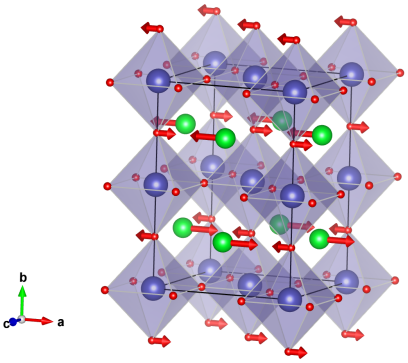


Figure 8. X5- distortion mode in the Pnma structure of SrZrO3, as obtained with VESTA in the same way as the R5- distortion mode, explained in the text and shown in Figure 7.

Following a similar process, all the different symmetry distortion modes present in the structure can be visualized. Figure 8 shows the result for the X5- distortion mode, which has a much smaller amplitude than the R5- mode. In this case, the mode clearly implies a distortion of the ZrO_6 octahedra, while the Sr atoms exhibit correlated displacements. Notice that the relative values of the displacements of the Sr atoms and the apical oxygens in the octahedra are not forced by the symmetry of the mode, and come from the experimental structure.

The creation of an ".mcif" to be subsequently used and visualized using VESTA is the most robust and flexible user-friendly method for the visualization of the modes determined by AMPLIMODES. However, STRCONVERT can also directly create (by clicking on "Export to VESTA format (displacement)") a VESTA file to be loaded in this program (see Figure 3). This VESTA file describes the non-distorted reference structure without symmetry (space group P1), listing all atomic positions within a unit cell corresponding to the high symmetry parent structure, and includes all non-zero atomic displacements of the mode as vectors. VESTA depicts graphically these vectors as arrows when visualizing the structure. The vectors are however associated to individual atoms, and not to "crystallographic sites". This implies that the depiction of the displacement vectors of the mode is restricted to the atoms within one unit cell, and the mode cannot be visualized in regions comprising more than one unit cell.

In addition, STRCONVERT has a built-in JSmol plugin (button "visualize (displacement)" in Figure 3) to visualize the mode directly in the browser with JSmol (look for the link to the visualization at the bottom of the resulting webpage after clicking on the mentioned button). The available menu on the resulting webpage is however quite limited. In order to have some additional flexibility on the editing of the image, specific commands must be entered on the console that can be opened by making use of the menu available by right-clicking on the JSmol image.

JSmol mimics Jmol, and the available commands are the same for the two programs. For the visualization capabilities attained with some commands of JSmol, please, see next section, where the visualization using directly Jmol is explained, and a set of basic commands of the program are presented.

In fact, as stressed below, the procedure for a locally installed Jmol program, which is explained in the next section, could also be followed with JSmol, made available in the visualization webpage of STRCONVERT.

4. Visualizing the distortion symmetry modes with Jmol

The output of AMPLIMODES in the form of a html file, as the one we have previously saved, with the name modes_SrZrO3.html, can be directly loaded in Jmol. This program directly interprets this html file and creates a distinct "frame" or visualized structure for each distortion mode (see Figure 9), and also for the high-symmetry and low symmetry structures being compared (both in the basis of the low symmetry space group, as listed in the output of AMPLIMODES).

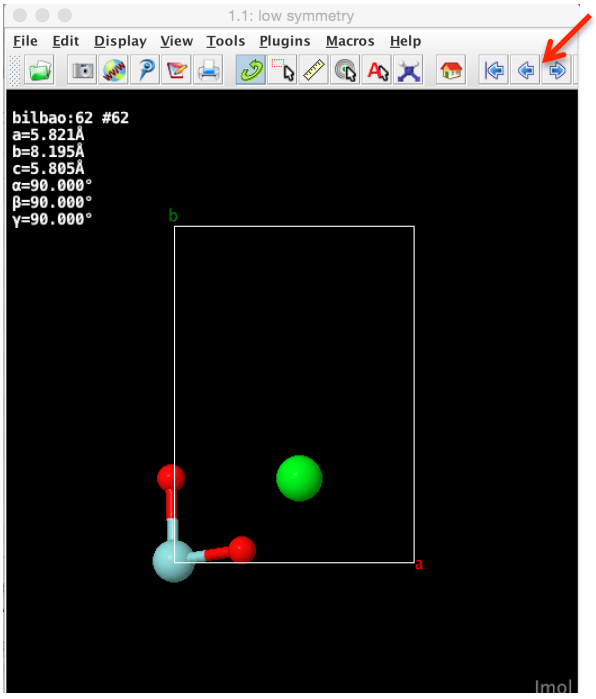


Figure 9. Aspect of the window of Jmol after loading the html file containing the output of AMPLIMODES for the *Pnma* structure of $SrZrO_3$. The different frames/structures representing the the low and high symmetry structures and each distortion mode can be seen using the arrows on the heading of the window, highlighted with a red arrow.

The program only shows the atoms of the asymmetric unit of each structure, which in the case of the frames associated with the distortion symmetry modes is the high-symmetry non-distorted structure, described in the low-symmetry setting.

The program Jmol has an infinity of possibilities for editing each of the frames and achieving a visualization according to the wishes of the user. A full exploitation of these possibilities would be achieved by introducing adequate commands in the console that can be opened from the menu obtained by right-clicking on the Jmol window (see Figure 10). However, for a user not familiar with the program, this requires considerable intensive effort in the study of the program manual and the help tools of the program. Here we will limit ourselves to indicate the most simple steps to obtain aceptable graphical depictions of the distortion symmetry modes both in a static and in a dynamic form.

Incidentally, if Jmol is not available or if for any reason the user does not wish to have a local installation of this Java program, a similar visualization can be achieved using the JSmol in the webpage opened by the button: "visualize (displacement)", shown in Figure 3. Once the visualization webpage is opened with a JSmol window, it is sufficient to drag the html file with the output of AMPLIMODES on the JSmol window. We can then follow similar steps as those indicated below for a local Jmol.

The first thing is to make the program depict all the atoms within a unit cell. To do this right-click to develop the menu shown in Figure 10, and choose the option "Symmetry", and there the option: "reload {444 666 1} + Display 555". The resulting visualization for some of the frames is shown in Figure 11.

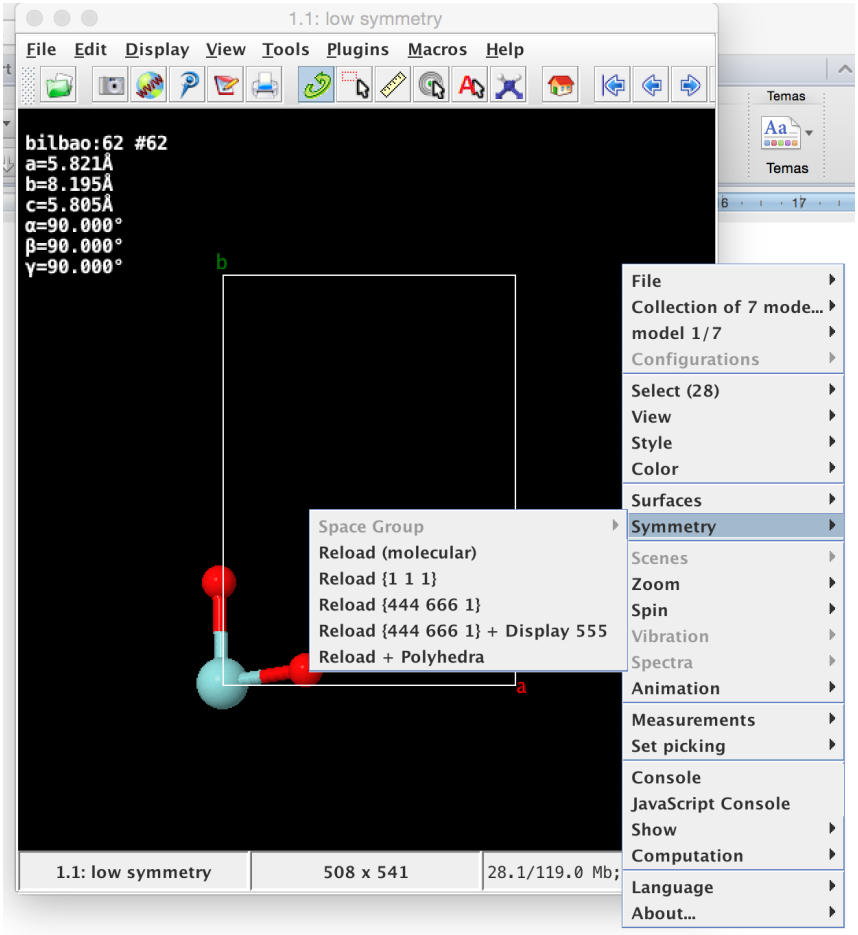


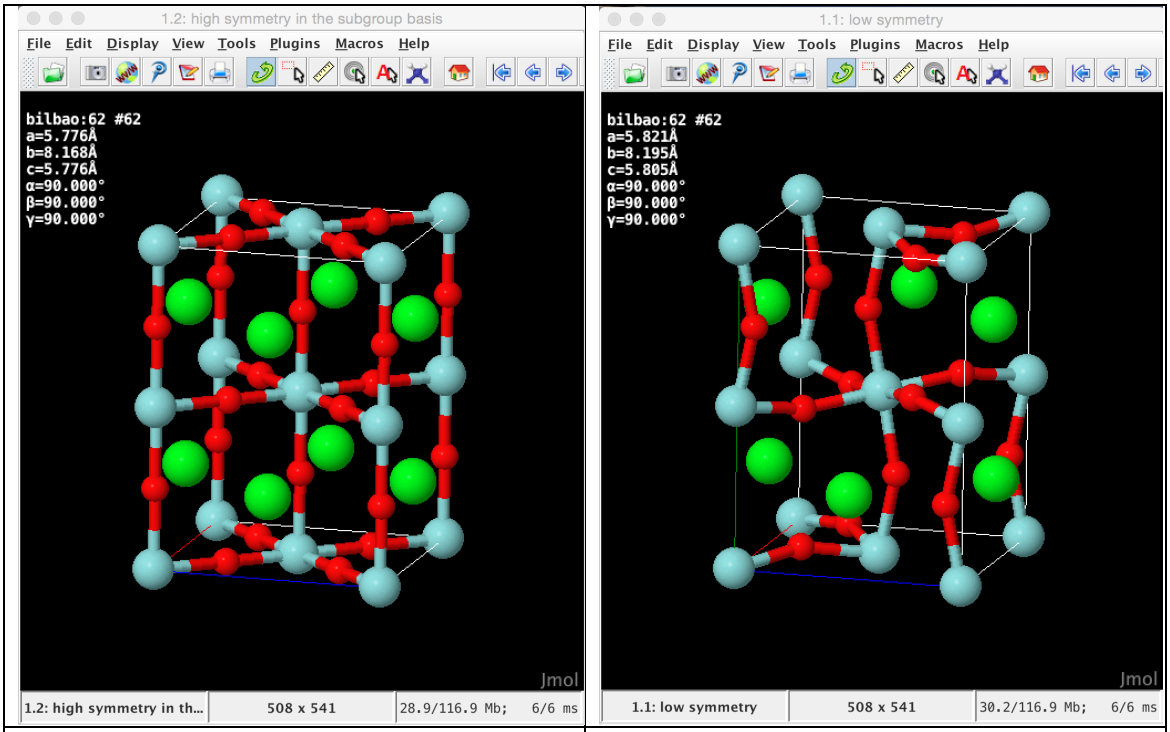
Figure 10. Screenshot showing the right-click menu and the "symmetry" optional reloads to depict a full unit cell. A direct command of type: "load "" {1,1,1} packed" on the console can also be used to visualize all atoms within a unit cell.

A more flexible depiction of the frames, including all atoms within a unit cell can be done by opening the cnsole in the right-click menu, and introducing the command:

load "" {1,1,1} packed

The program will then depict all atoms in one unit cell including those on the edges, similarly as in Figure 11. If one wishes to visualize a region comprising several unit cells, say for instance a volume 2x2x2 in terms of unit cells along the three cell directions, it is sufficient to substitute {1,1,1} in the command above by {2,2,2}.

At this stage, the frames corresponding to the distortion modes, all depict the same structure, namely the high-symmetry one shown in Figure 11(a). The actual depiction of the distortion symmetry modes in each frame requires some additional commands, which depend on whether we wish to visualize the mode in a statical or in a dynamical form.



(a) (b)

Figure 11. High (a) and low symmetry (b) structures of $SrZrO_3$ after using the option: symmetry -> reload {444 666 1} + Display 555 on the right-click menú shown in Figure 10

- Visualization of the modes in a static form:

This is a depiction analogous to the one that we obtained above using STRCONVERT and VESTA. The mode is represented by vectors on each atom proportional to the corresponding atomic displacement associated with the mode. In order to do that we introduce in the console the commands:

vectors on
vector scale 5
vector 0.07

The last two commands, controlling the scale and the width of the vectors, can be changed according to necessity for the representation of each mode. Figure 12 shows the results for the R5- and the M2+ distortion modes.

One can readily switch now to a visualization with explicit ZrO_6 octahedra. This requires the inclusion of atoms outside the unit cell and can be done with the command:

load “” {1,1,1} packed 0.3

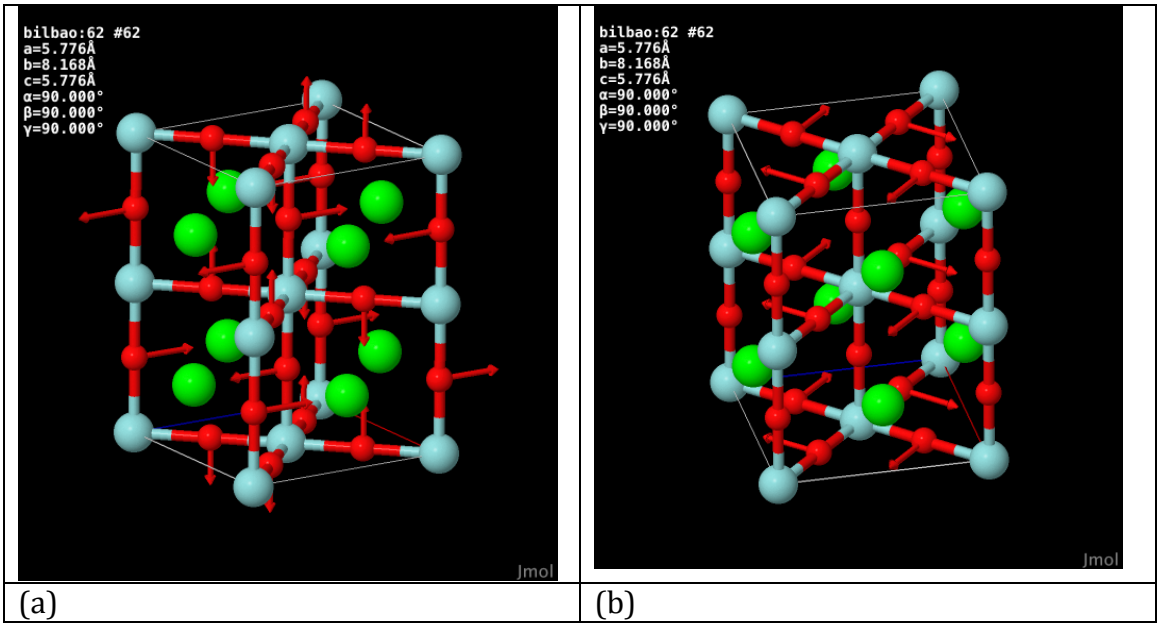


Figure 12. R5- (a) and M2- (b) distortion modes in the *Pnma* structure of $SrZrO_3$ obtained after using the vector editing commands.

The addition of the value "0.3" implies now that all atoms outside the unit cell but in an interval of 0.3 for the distance in terms of the components along the three axes, are also included. This is sufficient to include the oxygens outside the unit cell belonging to the ZrO_6 octahedra. The editing commands mentioned above concerning the displacement vectors have now been obliterated and must be introduced again. The result for the R5- mode is shown in Figure 13(a). A simpler picture with a framework of octahedra is obtained with the command:

```
polyhedra
set showUnitCellInfo false
```

This is shown in Figure 13(b). The second command deletes the text heading on the image. Finally with the commands:

```
color polyhedra translucent
connect delete
```

the polyhedra are made translucent and the bond framework is deleted as shown in Figure 14. Images can be saved in different formats using the "File" button on the heading bar of the program window: File →Export →Export image.

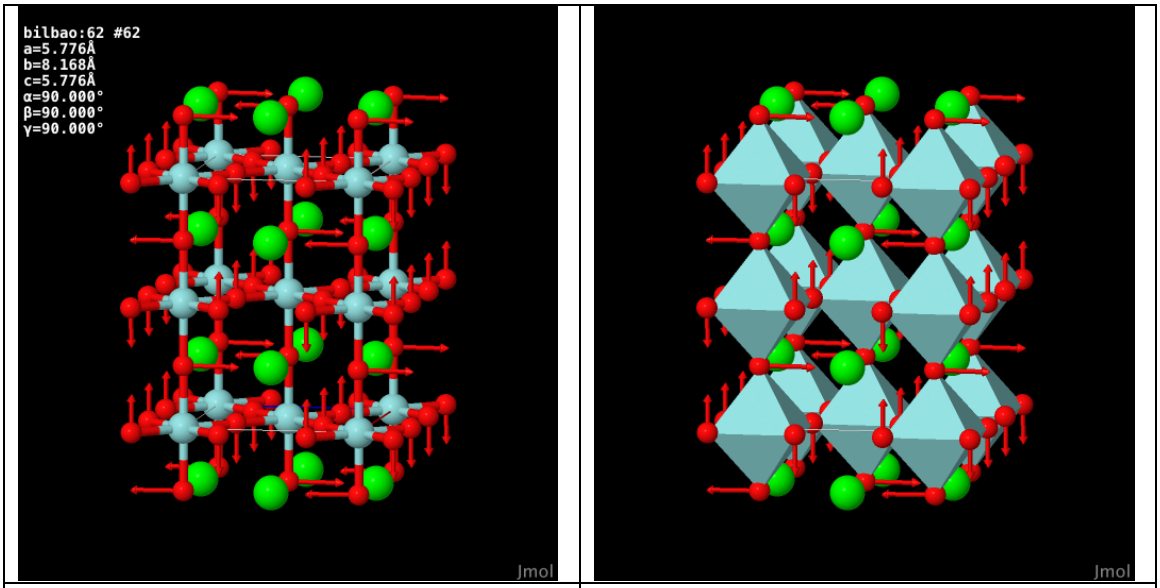


Figure 13. (a) R5- distortion mode showing the correlated movements of the ZrO3 octahedra.(b) The same after the command "polyhedra".

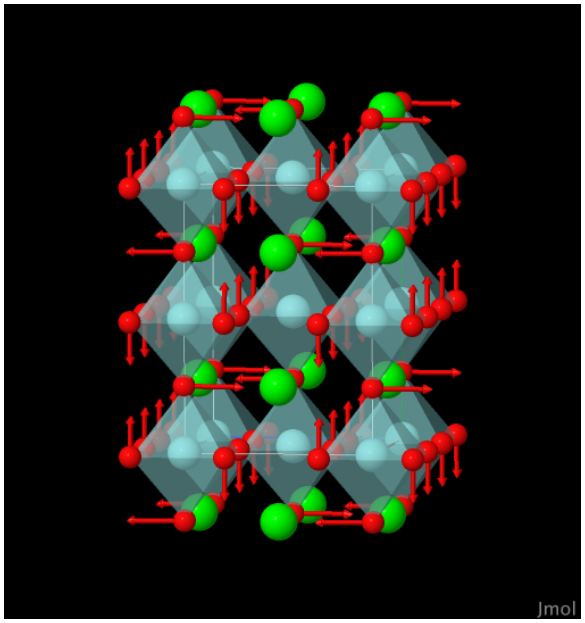


Figure 14. R5- distortion mode after further editing with "color polyhedra translucent" and "connect delete".

- *Visualization of the modes in a dynamic form:*

Instead of using arrows, Jmol can depict the distortion modes as a vibrational mode, showing the vibration as an endless periodic movement, with a period that can be adjusted by the user. Short movies gif format can then be produced of this dynamic representation of the distortion modes. Here the most simple steps to achieve that.

We delete the depiction of displacement vectors and we activate the vibration option:

vectors off
vibration on

This latter step can also be done using the right-click menu. The period and amplitude of the dynamic vibrations can be controlled with the commands:

vibration period 3
vibration scale 2

We can delete the translucent feature of the polyhedra by just commanding again:

polyhedra

The resulting dynamic visualization is shown in Figure 15 for the R5- and X5- distortion modes. These .mov animations have been obtained by direct transformation of the gif files created by Jmol with commands such as the following ones:

animation mode loop
capture "R5-_vibration.gif" 5.0

By default the created gif file is saved with the chosen title in the directory of the Jmol program. In order to save it in other directory, the whole file address should be given as file name.

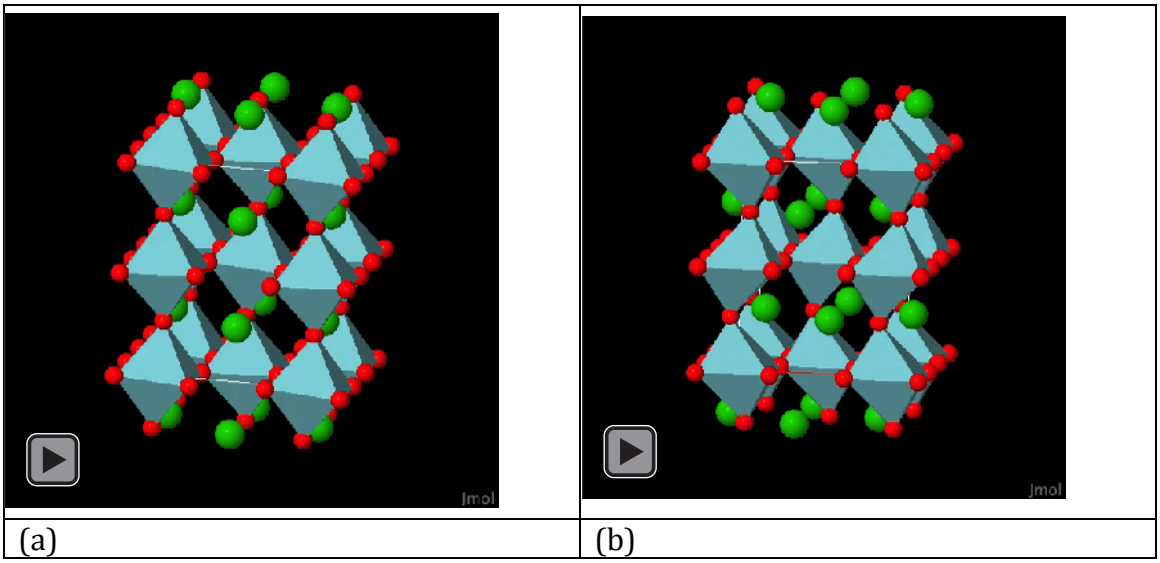


Figure 15. Animation of the R5- (a) and the X5- distortion modes that are present in the *Pnma* structure of $SrZrO_3$, as obtained with Jmol. The original files created by the program are in GIF format.

By introducing:

polyhedra off
connect

we can recover the visualization of the bonding framework, and see the modes under this scheme. Figure 16 shows the animation obtained for the M2+ distortion mode, the second largest in the *Pnma* structure of $SrZrO_3$, which also corresponds to a rigid unit mode of the ZrO_6 octahedra.

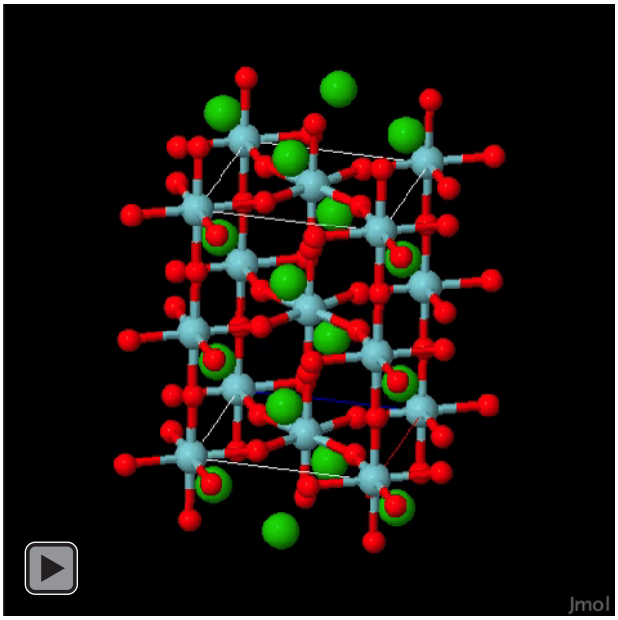
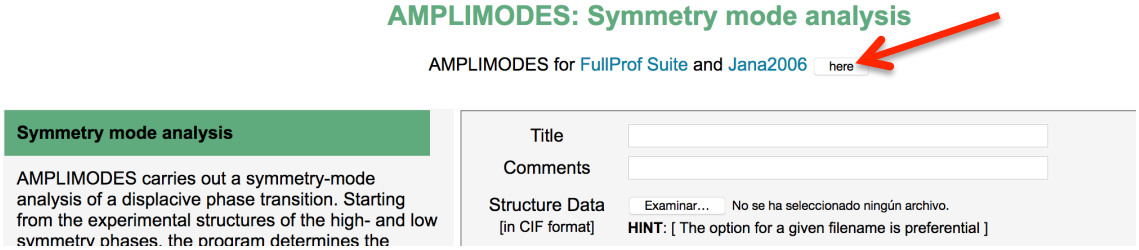


Figure 16. Animation of the M2+ distortion mode that is present in the *Pnma* structure of $SrZrO_3$, as obtained with Jmol. The original file created by the program is in GIF format.

5. Visualizing the distortion symmetry modes with FullProf and VESTA

AMPLIMODES can transform its output into a format (PCR file) that can be directly loaded into FullProf [10] for a powder neutron diffraction simulation. If experimental data is available, some further small editing of this PCR file is sufficient to make FullProf ready for a refinement of the low-symmetry structure, where, the amplitudes of the symmetry-adapted modes are refinement parameters, instead of the individual atomic coordinates. However, for our purposes, the important feature of FullProf when executed with a PCR file created by AMPLIMODES is its automatic creation of a set of files intended for the visualization of all the distortion symmetry modes in the structure.

Let us explain this feature using the same case study that has been considered in the previous sections. First, when opening the webpage of AMPLIMODES we must switch to the FullProf option by clicking at the top on the "AMPLIMODES for FullProf and JANA" button:



The input webpage is then changed to a similar one, where the introduction of the full data for the low symmetry structure is optional, its space group and the setting transformation being the only necessary input, apart from the high temperature structure. This is very important, because it means that the program can be used without any quantitative knowledge of the low-symmetry structure, except for its space group and the relation of its setting with the one of the parent structure. In this case, the program can be used to visualize all the symmetry modes that can be involved in the distorted structure, without any knowledge of the specific mode combination that describes the actual distortion present in the structure.

For our example, we introduce as in section 2 the high and low temperature structures in the appropriate windows or upload the corresponding CIF files, and type the setting transformation indicated in section 2. After submission, AMPLIMODES provides an output webpage similar to the one obtained in section 2, but at the bottom some text lines appear:

You can copy and paste the following text on your .pcr file

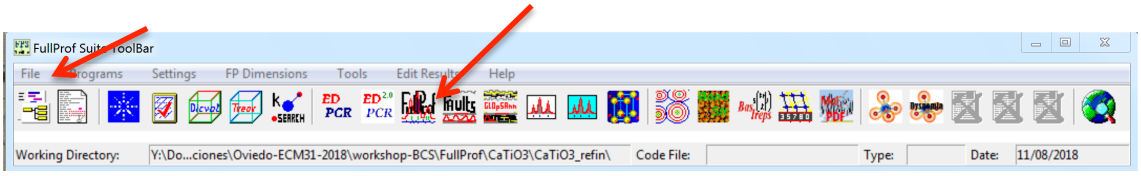
```
062                    <--Space group symbol
!Atom   Typ       X         Y         Z      Biso      Occ      In Fin N_t Spc /Codes
Sr1     SR      0.500000  0.750000  0.000000 0.500000 0.500000  0   0   0    1
                  0.00      0.00      0.00     0.00     0.00
Zr1     ZR      0.000000  0.000000  0.000000 0.500000 0.500000  0   0   0    1
                  0.00      0.00      0.00     0.00     0.00
O1      O       0.750000  0.000000  0.250000 0.500000 1.000000  0   0   0    1
                  0.00      0.00      0.00     0.00     0.00
O1_2    O       0.500000  0.250000  0.500000 0.500000 0.500000  0   0   0    1
                  0.00      0.00      0.00     0.00     0.00
! Polarisation Vectors of Symmetry Modes for each atom
V_MODES   12
! Nm Atm     Irrep      Vx        Vy        Vz         Coeff
  1 Sr1     R4-      0.000000  0.000000  0.086570 1.00
  2 O1      R4-      0.000000  0.030607  0.000000 1.00
  2 O1_2    R4-      0.000000  0.000000 -0.061214 1.00
  3 O1      R5-      0.000000  0.030607  0.000000 1.00
  3 O1_2    R5-      0.000000  0.000000  0.061214 1.00
  4 Sr1     X5-     -0.086570  0.000000  0.000000 1.00
  5 O1      X5-      0.000000  0.000000  0.000000 1.00
  5 O1_2    X5-     -0.086570  0.000000  0.000000 1.00
  6 O1      M2+     -0.043285  0.000000 -0.043285 1.00
  6 O1_2    M2+      0.000000  0.000000  0.000000 1.00
  7 O1      M3+     -0.043285  0.000000  0.043285 1.00
  7 O1_2    M3+      0.000000  0.000000  0.000000 1.00
!Amplitudes of Symmetry Modes
A_MODES    7   2
    A1_R4-   -0.046206     1.00
    A2_R4-    0.024504     1.00
    A3_R5-    1.151688     1.00
    A4_X5-    0.277232     1.00
    A5_X5-    0.150166     1.00
    A6_M2+   -0.797040     1.00
    A7_M3+    0.011552     1.00
```

You can download the full .pcr file for a default neutron simulation here

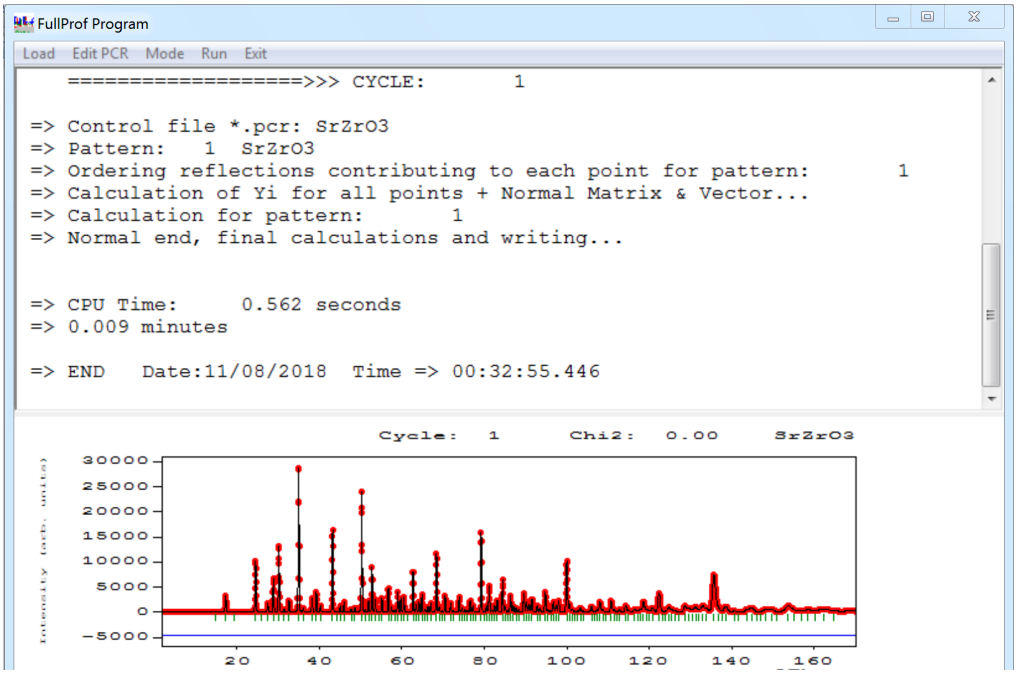
We can read at the bottom, the amplitudes of the seven symmetry modes determined by AMPLIMODES. If the information on the low-symmetry structure had been limited to the space group, these amplitudes would have appeared with null values.

Just click on the indicated button at the bottom of the text output to download a .pcr file for a default neutron simulation. In some browsers the resulting file appears then on the browser window. We save it with the name SrZrO3.pcr.

We open now the FullProf Suite toolbar:



On the option "File", we select the working directory where all files created by FullProf will be saved and the input SrZrO3.pcr file has been saved. We open subsequently the console of the FullProf program and load the mentioned .pcr file. FullProf calculates then and shows a simulated neutron powder diffraction diagram of a structure with the symmetry modes having the amplitudes given in the .pcr file:



During execution, the program has also created for each of the distortion symmetry modes two files intended for their visualization. These files can be found in the working directory. One of them is a .vesta file that can be directly loaded in VESTA [7]. Figure 17 shows the resulting direct visualization of this file for the particular case of the R5- distortion mode (file name: SrZrO3_Irrep_R5-.vesta). VESTA is a very user-friendly program where further editing can be readily done to transform this first image into one similar to that shown in Figure 7.

Thus, FullProf creates in a single run an initial .vesta file for each distortion mode in the low-symmetry structure. It is important to note that these .vesta files are all linked to a single CIF file (in our case: SrZrO3_parent.cif), also created by FullProf, which describes the parent high-symmetry structure, which is taken as reference for all modes. The mode .vesta files will not work without the presence in the same directory of this .cif file. It is also to be noted that these files require for a proper visualization that at least one of the symmetry modes associated with the corresponding irrep has a non-zero amplitude in the input .pcr file.

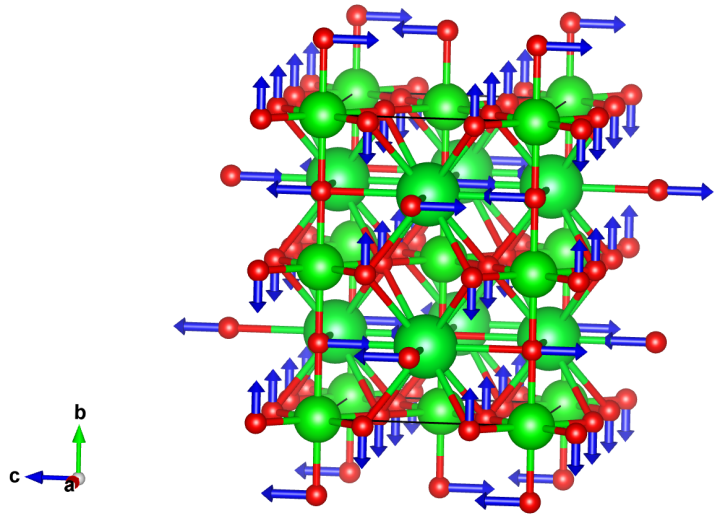


Figure 17. Direct visualization with VESTA with no additional editing of the .vesta file created by FullProf for the R5- distortion mode.

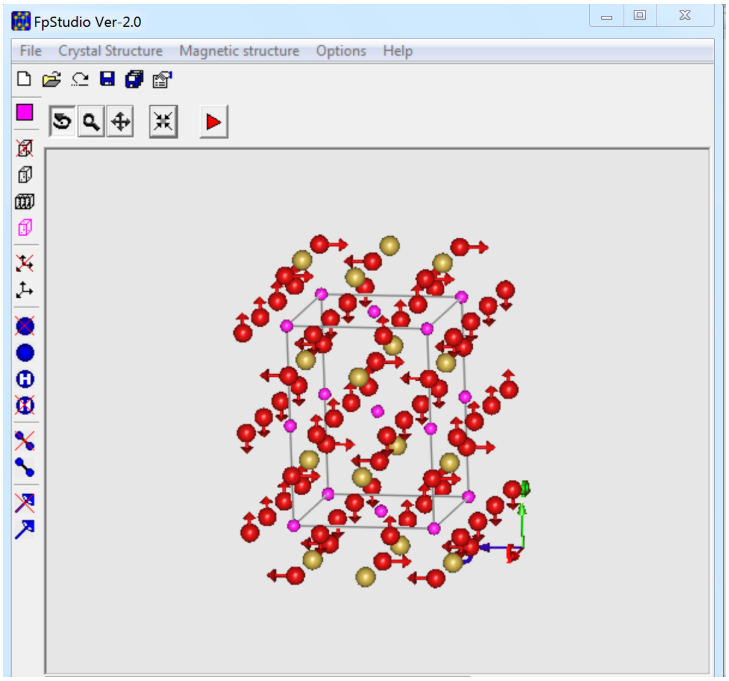


Figure 18. Direct visualization with FpStudio, with no editing, of the .fst file created by FullProf for the R5- distortion mode.

The second alternative file for visualization purposes created by FullProf for each distortion symmetry mode has the extension .fst and is intended for the program FpStudio, which is part of the FullProf Suite. This program can be readily activated by clicking on the corresponding icon of the Fullprof Suite toolbar. Figure 18 shows the result when loading file with name: SrZrO3_1_Irrep_R5-.fst, corresponding to the R5- distortion mode. This first visualization can be improved with appropriate editing of the .fst file, but this in general requires getting deep

into the particular features of FpStudio and the possible commands that can be introduced in a .fst file, through a careful study of the manual program.

References

[1] Danel Orobengoa, Cesar Capillas, Mois I. Aroyo, and J. Manuel Perez-Mato. AMPLIMODES: symmetry-mode analysis on the Bilbao Crystallographic Server. Journal of Applied Crystallography, 42(5):820_833, Oct 2009.

[2] J. M. Perez-Mato, D. Orobengoa, and M. I. Aroyo. Mode crystallography of distorted structures. Acta Crystallographica Section A, 66(5):558_590, Sep 2010.

[3] M.I. Aroyo, J.M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov, and H. Wondratschek. Bilbao crystallographic server: I. databases and crystallographic computing programs. Zeitschrift fur Kristallographie, 221(1):15_27, 2006.

[4] Mois I. Aroyo, Asen Kirov, Cesar Capillas, J. M. Perez-Mato, and Hans Wondratschek. Bilbao Crystallographic Server. II. Representations of crystallographic point groups and space groups. Acta Crystallographica Section A, 62(2):115_128, Mar 2006.

[5] M.I. Aroyo, J.M. Perez-Mato, D. Orobengoa, E. Tasci, G. De La Flor, and A. Kirov. Crystallography online: Bilbao crystallographic server. Bulgarian Chemical Communications, 43(2):183_197, 2011.

[6] Branton J. Campbell, Harold T. Stokes, David E. Tanner, and Dorian M. Hatch. ISODISPLACE: a web-based tool for exploring structural distortions. Journal of Applied Crystallography, 39(4):607_ 614, Aug 2006.

[7] Koichi Momma and Fujio Izumi. VESTA3 for three-dimensional visualization of crystal, volumetric and morphology data. Journal of Applied Crystallography, 44(6):1272_1276, Dec. 2011.

[8] Hanson R. 2013. *Jmol: an open-source Java viewer for chemical structures in 3D*. http://www.jmol.org/

[9] Perez-Mato, J. M., Gallego, S. V., Tasci, E. S., Elcoro, L., de la Flor, G. and Aroyo, M. I. (2015). Annu. Rev. Mater. Res. 45, 217–248.

[10] Rodriguez-Carvajal J. 1993. *Physica B* 192:55–69