$Cs_2AgInCl_6$ is a halide perovskite material that is used in solar energy conversion or light-emitting diodes. Crystallographic Information File (CIF) of this material is given along with this assignment.

(1) Load the CIF file of $Cs_2AgInCl_6$ in Vesta software. If you have not installed Vesta please use the following link and install the software.
https://jp-minerals.org/vesta/en/download.html

These questions are given for you to familiarize yourself with Vesta software and basic crystallographic properties.

After you load the file (in Ball- and –stick mode), carefully visualize the structure, identify all the atoms and answer the following questions.

a. Identify the coordination number of Ag, In and Cs.
b. Identify the bond lengths of Ag-Cl, In-Cl and Cs-Cl. If more than one bond is present for any given cation, identify if all the bond lengths are same.

For each of the questions from c-i, export the images (with their axis) of the resulting crystal structures and copy them in your assignment.

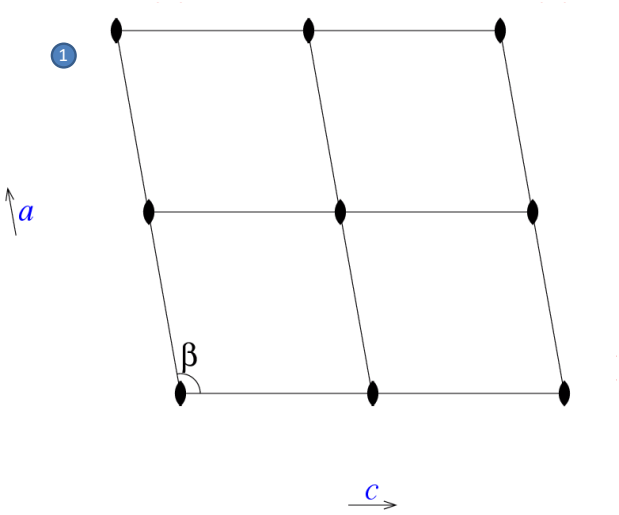
c. If the bond length is greater than 3Å, hide those bonds.
d. Convert the structure from ball-and-stick mode to polyhedral mode
e. Hide Cs atoms from the polyhedral structure shown in (d). Visualize the narrow pores formed in the resulting structure.
f. Identify the unit cell (hint: use options in Properties dialog box; try hiding bonds and polyhedra). Locate and give the coordinates of all the cations present in the unit cell. Identify the total number of Ag, In, Cl and Cs atoms present in the unit cell. Verify if it matches with the stoichiometry $Cs_2AgInCl_6$.
g. Load the CIF file again and generate (100), (010) and (001) planes. Identify the atoms in these planes and see if they belong to the same family of planes.
h. When you load the CIF file by default (x,y,z) min is set to (0,0,0) and max is set to (1,1,1). Change the minimum to (-1,-1,-1). Generate all the family of planes corresponding to <0 -1 0>. Copy the necessary images so that I can see all the planes associated with this family.
i. Generate a plane (101) and compare the distance and angle between various atoms. Similarly generate (100) plane and find bond distances/angles. Explain if you find any difference in angles/distances between the same set of atoms in these two planes.

(2) Open the CIF file using notepad and carefully go through the file.

a. From the CIF file identify and give all the cell parameters. Check if the values identified in the CIF file match with the measured lattice parameters in Vesta. Identify and give the space group in which the material crystallizes in. Explain the space group symbol in detail. All the components need to be clearly explained, along with the type of crystal system, point group and centering.
b. From the link below identify the space group number corresponding to the space group of $Cs_2AgInCl_6$.
http://img.chem.ucl.ac.uk/sgp/large/sgp.htm
Click the corresponding space group and load the space group diagram.

From the space group diagram identify and give the name of all the symmetry operations (to understand the symmetry symbols use the following link: http://img.chem.ucl.ac.uk/sgp/misc/symbols.htm)

(3) Below is a space group diagram. An atom labeled '1' is given. Generate all the other atoms in the diagram.



(4) X-ray Diffraction

a. Load the CIF file of $Cs_2AgInCl_6$ in Vesta. Simulate the X-ray diffraction pattern. (Make sure to use the correct X-ray source wavelength as given in the CIF file). In the simulated plot, identity the reflection (hkl) planes of all the major peaks between 20 and 60° and label them.

b. (export the generated X-ray diffraction pattern to excel from File menu in the Powder Diffraction Pattern window)
The material $Cs_2AgInCl_6$ is manipulated inorder to tune the optical properties. The In^{3+} cation is substituted with Bi^{3+} and the new material takes the formula $Cs_2AgIn_xBi_{1-x}Cl_6$.
The materials with x=0,0.2,0.4, 0.6, 0.8 and 1 are synthesized in our laboratory. These materials are characterized using X-ray diffraction and the measured data is given in the attached excel sheet in this assignment folder. (File name: xrd.xlsx). Compare the simulated XRD pattern in 4(a) and the experimentally measured pattern of $Cs_2AgInCl_6$. If any difference is found find the lattice parameter a, b and c for the experimentally measured XRD pattern of $Cs_2AgInCl_6$. (Hint: consider normalizing the simulated XRD pattern and the measured patterns to enhance the ease of comparison)

c. Find the lattice parameters a, b, c for all values of x. Plot 'a' as a function 'x'. If any variations are observed, explain why the substitution of In^{3+} by Bi^{3+} introduced a change in the lattice parameters.

(5) Defects: Write the Kroger-Vink notation for the following conditions and explain the type of conductivity introduced.

a. Substitution of In^{3+} by Bi^{3+} in $Cs_2AgInCl_6$.

b. Introduce Bi^{3+} in the interstitial site of $Cs_2AgInCl_6$

c. Vacancy of anion

d. Vacancy of Ag^{+} cation
e. Substitution of In^{3+} by Mg^{2+}