1. The feature extraction part done is completely wrong

I have implemented code for feature extraction please run that, I am attaching it.

2. The model is not right as well. Please do the following steps for the model.
   Total number of atoms in a crystal is equal to max(Bar_connectivity_i_j) for a given crystal. For example in the first crystal max(Bar_connectivity_i_j)=8, there are 8 atoms. Nodal connectivity of each atom is the number of times is occurs in the bar connectivity column. For the first datapoint each atom occurs thrice in the bar_connectivity so the node connectivity of each node/atom is 3.
   Total number of edges in the crystal is max(i in the bar connectivity_i_j).
   For example in the first one it is 12.
   Features extracted from each edge are 4 (length, l, m, n)
   Form a convolution layer for each atom using

$$\boldsymbol{v}_i^{(t+1)} = \mathrm{Conv}\left(\boldsymbol{v}_i^{(t)}, \boldsymbol{v}_j^{(t)}, \boldsymbol{u}_{(i,j)_k}\right), \quad (i,j)_k \in \mathcal{G}. \quad (1)$$

   Where in this formula i is the first atom, j is the 2nd atom and u(i,j) contains the properties of the edge connecting it. For example in the first dataset first edge bar_connectivity_1_1 and bar_connectivity_1_2 signifies that first edge is between 1st and 5th atom so 1st feature vector formed is
   (nodal connectivity(1),nodal connectivity(5), edge features(1st edge formed by 1 and 5)) == (3, 3, (length of edge between 1 and 5, l, m,n))
   Similarly do it for all edges. Total number of feature vectors for a given crystal would be equal to the total number of edges of the crystal.

Form a graph using node and edge parameters as given above by applying CNN with 20 layers and further create the entire CGCNN model with 30,40 Hidden layers and pooling layers as mentioned on the page 1,2,3 of the pdf named “cgcnn” attached. Do hyperparameter tuning in the hidden layer changing various functions so as to increase accuracy of model atleast above 90 percent.

Report-

1. Accuracies/errors of the model in predicting the given properties.
2. Function that takes input of nodal positions, bar connectivity, a,b,c,alpha,beta,gamma as input and predits the properties Cx, Cy, Cz and nx, ny, nz with the accuracy more than 90 percent.
3. Plot of Y predicted vs Y true
4. Error plot
5. Summary/ documentation of the model