**Exercise8 Web App for Symmetry Equivalent Molecules generation using PHP**

Aim : To create a web app for symmetry equivalent molecules generation using PHP

Learning Outcome:

* **The student will be able to use file handling concepts using PHP**
* **Also student will be able to understand the regular expression syntaxes in PHP scripts**

**Procedure**

* **Load a CIF molecule in the server using HTML form**
* **Input the Symmetry operation using Input box**
* **Develop a PHP script in web server for finding the symmetry equivalent molecules**

**Example: CIF file**

**#######################################################################**

**#**

**# Cambridge Crystallographic Data Centre**

**# CCDC**

**#**

**#######################################################################**

**#**

**# If this CIF has been generated from an entry in the Cambridge**

**# Structural Database, then it will include bibliographic, chemical,**

**# crystal, experimental, refinement or atomic coordinate data resulting**

**# from the CCDC's data processing and validation procedures.**

**#**

**#######################################################################**

**data\_test1 in P2(1)/c**

**\_symmetry\_cell\_setting monoclinic**

**\_symmetry\_space\_group\_name\_H-M 'P 21/c'**

**\_symmetry\_Int\_Tables\_number 14**

**\_space\_group\_name\_Hall '-P 2ybc'**

**loop\_**

**\_symmetry\_equiv\_pos\_site\_id**

**\_symmetry\_equiv\_pos\_as\_xyz**

**1 x,y,z**

**2 -x,1/2+y,1/2-z**

**3 -x,-y,-z**

**4 x,1/2-y,1/2+z**

**\_cell\_length\_a 13.0811(4)**

**\_cell\_length\_b 12.5251(3)**

**\_cell\_length\_c 14.2042(5)**

**\_cell\_angle\_alpha 90**

**\_cell\_angle\_beta 114.730(4)**

**\_cell\_angle\_gamma 90**

**\_cell\_volume 2113.81**

**loop\_**

**\_atom\_site\_label**

**\_atom\_site\_type\_symbol**

**\_atom\_site\_fract\_x**

**\_atom\_site\_fract\_y**

**\_atom\_site\_fract\_z**

**O5 O 0.456822 -0.058695 0.316797**

**N1 N 0.946565 0.498009 0.221943**

**Generating Symmetry Equivalent molecules**

* **For the Nitrogen atom given below take x,y and z co-ordinates .**

**N1 N 0.946565 0.498009 0.221943**

* **Assume the Symmetry Operation is : -x,-y,-z**
* **Applying this operation to the above x,y and z co-ordinates of Nitrogen atom ( chaging the sign of the atom co-ordinates )we will get the new set of x,y and z co-ordinates for the Nitrogen as follows :**

**N1 N -0.946565 -0.498009 -0.221943**