**Exercise 7 :Characterization of interactions(Hbond or Van der Waals) using PHP scripts**

**Aim:** To know the nature of interactions in crystallized molecules using PHP scripts.

Presence of a bond critical point (BCP) between interacting atoms

Koch and Popelier condition deals with the mutual penetration of the hydrogen and the acceptor atom.

**r0D – Non-bonded radii of donor(vdw)**

**r0A – Non-bonded radii of acceptor(vdw)**

**rD and rA : Bonding radii of donor and acceptor (distance)**

**ΔrD = (r0D – rD) > ΔrA = (r0A – rA) and rD + rA > o**

**For hydrogen bonding character: if two conditions are satisfied**

**For van der Waals type: if either or both of these conditions are violated**

**Given :** The following data are retrieved from Quantum statistics analysis

|  |
| --- |
| Br 1.54E+01 5.81E+00 1.40E+01  B1 1.58E+01 7.64E+00 1.31E+01  Br 1.62E+01 9.47E+00 1.23E+01 |

* **First Line corresponds to first atoms**
* **Second Line corresponds to BCP**
* **Third Line corresponds to the second atom**

**Algorithm :**

1. Read the file using PHP file open syntax.
2. The co-ordinates are in the Scientific notation. Convert it to engineering notation

Example :

1. **1.54E+01 can be converted to 15.4.**
2. **1.54E-01 can be converted to 0.154**

**Use PHP syntax:**

**<?php**

**$number =1.54E-01 ;**

**$txt = sprintf("%f",$number);**

**echo $txt;**

**?>**

1. Find the Euclidian distance between the atoms (Br and B1) , (B1 and Br) and save the distances as variable newdist .The value of the distance is in Bohr radius.
2. Change the Bohr radius value into Angstroms using the formula given below and save it as ang\_dis

**1bohr radius =0.5292A°**

1. Use the following vanderwaal\_constants associative array and apply the following criteria.

**$vanderwaal\_constants =array("H"=>1.2,"C"=>1.70,"O"=>1.52,"N"=>1.55,"He"=>1.4,"F"=>1.47,**

**"Si"=>2.10,"P"=>1.80,"S"=>1.80,"Cl"=>1.75,"As"=>1.85,"Se"=>1.90,"Br"=>1.85,"Te"=>2.06,"I"=>1.98);**

1. Extract the value from the vanderWaal constant associative array for the atom Br. Then subtract the calculated distance between the first two atoms (Br,B) from the Vander Waal Constant value and assigned it as variable rd
2. Extract the value from the vanderWaal constant associative array for the atom Br. Then subtract the calculated distance between the second two atoms (B,Br) from the Vander Waal Constant value and assigned it as variable ra
3. Interpretation :

* If rd >ra , print a message saying **“Distance Criteria Satisfied”**
* If (rd+ra ) >0 and (rd-ra) >0 ,print the message **“Hydrogen Bond”** otherwise it is **“Van der Waaals”**