```
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 1.40
Initial guess for bond length-r2 of H2O(in Angstroms): 0.70
Initial guess for bond angle theta of H2O(in degrees): 120
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958       0.958      104.50143344]
Optimal Energy in (kJ/mol) =  7.202920254908353e-08


Time taken (in seconds) =  1.6881823539733887
Number of Basin-Hopping iterations =  1108
Number of Gradient Descent iterations =  356649
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 0.60
Initial guess for bond length-r2 of H2O(in Angstroms): 1.80
Initial guess for bond angle theta of H2O(in degrees): 90
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958       0.958      104.49856659]
Optimal Energy in (kJ/mol) =  7.202582761053294e-08


Time taken (in seconds) =  1.7165870666503906
Number of Basin-Hopping iterations =  1103
Number of Gradient Descent iterations =  354054
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 2
Initial guess for bond length-r2 of H2O(in Angstroms): 0.5
Initial guess for bond angle theta of H2O(in degrees): 130
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958       0.958      104.50143347]
Optimal Energy in (kJ/mol) =  7.20319009889804e-08


Time taken (in seconds) =  2.9198873043060303
Number of Basin-Hopping iterations =  1147
Number of Gradient Descent iterations =  376597
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 0.8
Initial guess for bond length-r2 of H2O(in Angstroms): 1.6
Initial guess for bond angle theta of H2O(in degrees): 150
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958      0.958     104.5014334]
Optimal Energy in (kJ/mol) =  7.202531316146585e-08


Time taken (in seconds) =  2.5257327556610107
Number of Basin-Hopping iterations =  1194
Number of Gradient Descent iterations =  399693
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 1.20
Initial guess for bond length-r2 of H2O(in Angstroms): 1.20
Initial guess for bond angle theta of H2O(in degrees): 80
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958       0.958      104.49856657]
Optimal Energy in (kJ/mol) =  7.202829251434903e-08


Time taken (in seconds) =  2.9160397052764893
Number of Basin-Hopping iterations =  1144
Number of Gradient Descent iterations =  374977
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(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 1.8
Initial guess for bond length-r2 of H2O(in Angstroms): 0.9
Initial guess for bond angle theta of H2O(in degrees): 100
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958        0.958      104.49856663]
Optimal Energy in (kJ/mol) =  7.202259934719246e-08


Time taken (in seconds) =  1.4816787242889404
Number of Basin-Hopping iterations =  1010
Number of Gradient Descent iterations =  307685
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 0.4
Initial guess for bond length-r2 of H2O(in Angstroms): 2.2
Initial guess for bond angle theta of H2O(in degrees): 140
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958        0.958      104.50143341]
Optimal Energy in (kJ/mol) =  7.20262490338393e-08


Time taken (in seconds) =  1.8562390804290771
Number of Basin-Hopping iterations =  1174
Number of Gradient Descent iterations =  389773
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 1
Initial guess for bond length-r2 of H2O(in Angstroms): 1.5
Initial guess for bond angle theta of H2O(in degrees): 95
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958        0.958      104.49856655]
Optimal Energy in (kJ/mol) =  7.202987064790966e-08


Time taken (in seconds) =  1.6178152561187744
Number of Basin-Hopping iterations =  1069
Number of Gradient Descent iterations =  337147
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 1.5
Initial guess for bond length-r2 of H2O(in Angstroms): 0.5
Initial guess for bond angle theta of H2O(in degrees): 100
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958        0.958      104.49856661]
Optimal Energy in (kJ/mol) =  7.2023833282153e-08


Time taken (in seconds) =  1.5144922733306885
Number of Basin-Hopping iterations =  1009
Number of Gradient Descent iterations =  307154
(base) PS C:\Users\swagg\OneDrive\Desktop\Desktop\Aaryan\IIITH\AAD\Project> python3 .\Basin-Hopping.py
Initial guess for bond length-r1 of H2O(in Angstroms): 0.7
Initial guess for bond length-r2 of H2O(in Angstroms): 1.9
Initial guess for bond angle theta of H2O(in degrees): 85
Optimal (r1,r2,theta) in Angstorm,degrees =  [  0.958        0.958      104.49856656]
Optimal Energy in (kJ/mol) =  7.202936626157277e-08


Time taken (in seconds) =  1.7530839443206787
Number of Basin-Hopping iterations =  1126
Number of Gradient Descent iterations =  365944
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