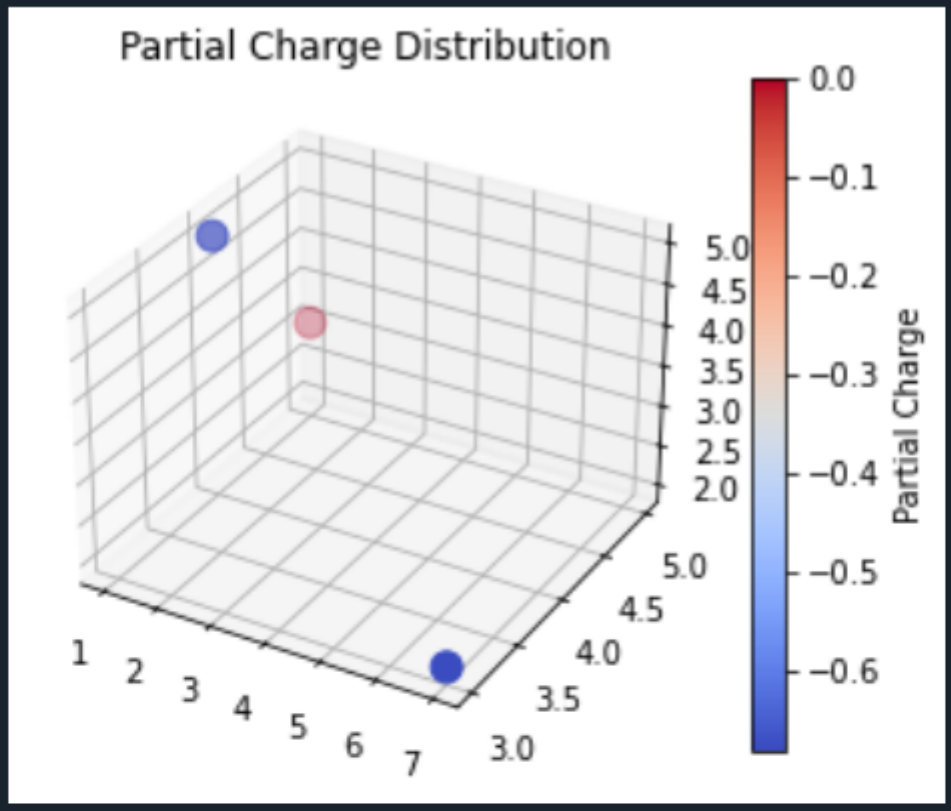


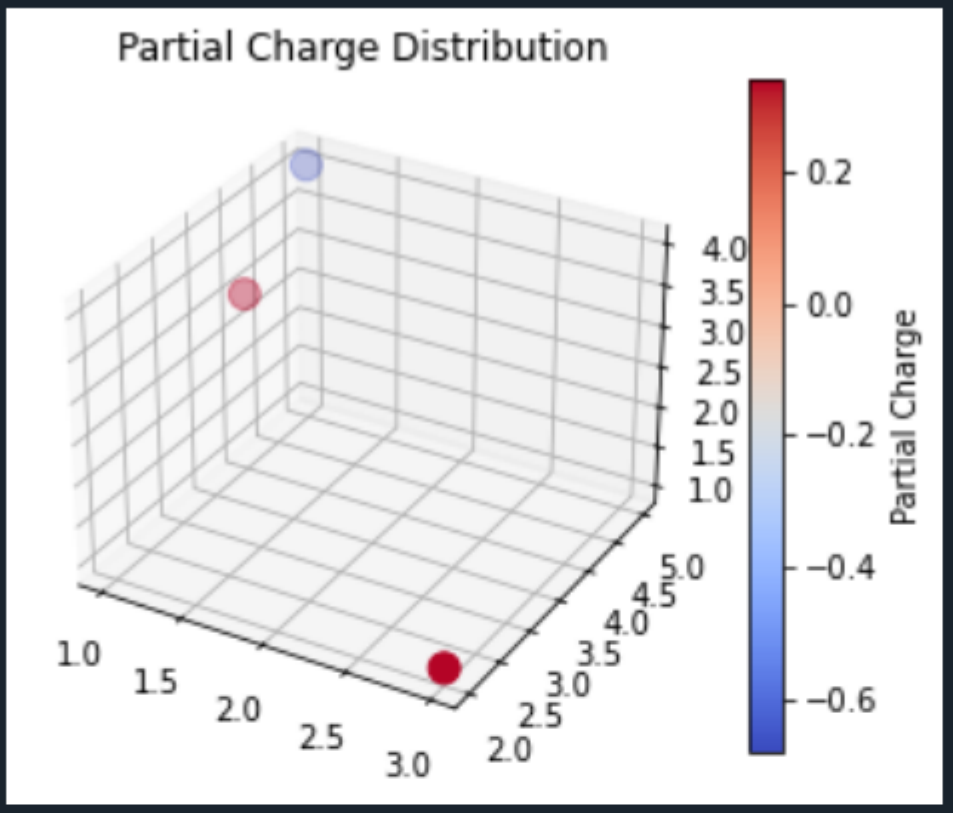
Help | Variable Explorer | Plots | Files

Console 1/A

```
In [2]: runfile('C:/Users/TANIYA/OneDrive/Desktop/Computational chemistry project.py', wdir='C:/Users/TANIYA/OneDrive/Desktop')
Enter the atoms in the molecule (e.g., H O H for H2O): C O O
Enter the 3D coordinates for C (x y z): 1 5 3
Enter the 3D coordinates for O (x y z): 7 3 2
Enter the 3D coordinates for O (x y z): 1 4 5

Bond Length between Atom 1 and Atom 2: 6.40 Å
Bond Length between Atom 2 and Atom 3: 6.78 Å
Bond Angle between Atom 1: 19.25°
Dipole Moment: [-5.44 -4.76 -4.76]
Electrostatic Potentials: [2.55, 3.44, 3.44]
Thermodynamic Properties: {'Molecular Weight (g/mol)': 44.009, 'Enthalpy (J/mol)': 1090.35466148, 'Entropy (J/mol·K)': 3.65890826}
```

IPython Console | History



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Console 1/A

```
In [3]: runfile('C:/Users/TANIYA/OneDrive/Desktop/Computational chemistry project.py', wdir='C:/Users/TANIYA/OneDrive/Desktop')
Enter the atoms in the molecule (e.g., H O H for H2O): H O H
Enter the 3D coordinates for H (x y z): 1 4 3
Enter the 3D coordinates for O (x y z): 1 5 4
Enter the 3D coordinates for H (x y z): 3 2 1

Bond Length between Atom 1 and Atom 2: 1.41 Å
Bond Length between Atom 2 and Atom 3: 4.69 Å
Bond Angle between Atom 1: 25.24°
Dipole Moment: [ 0.68 -1.36 -1.36]
Electrostatic Potentials: [2.2, 3.44, 2.2]
Thermodynamic Properties: {'Molecular Weight (g/mol)': 18.015, 'Enthalpy (J/mol)': 446.33459580000005, 'Entropy (J/mol·K)': 1.4977671000000001}
```

IPython Console | History