**Magnetic Behavior Python**

In this component, we will use Python to interface with Psi4, a quantum chemistry package, to calculate properties related to the magnetic behavior of different compounds. We will specifically focus on calculating the electron configuration, spin multiplicity, and magnetic susceptibility using quantum chemical methods.

**1. Setup and Installation:**

Before proceeding, ensure that both Psi4 and numpy are installed in your Python environment. You can install Psi4 using the following command:

pip **install** psi4

Install numpy as well, if not already available:

pip **install** numpy

**2. Python and Psi4 Script**

Here’s a Python script that uses Psi4 to compute the magnetic properties of a molecule:

**import** psi4  
**import** numpy **as** np  
  
# Set Psi4 memory and output file configuration  
psi4.set\_memory('500 MB')  
psi4.core.set\_output\_file('output.dat', False)  
  
# Define the molecule geometry (change this for different molecules)  
# Example: [FeCl3]  
molecule = psi4.geometry("""  
Fe 0.0000 0.0000 0.0000  
Cl 1.8000 1.8000 1.8000  
Cl -1.8000 -1.8000 1.8000  
Cl -1.8000 1.8000 -1.8000  
""")  
  
# Set the electronic structure method and basis set  
psi4.set\_options({  
 'reference': 'uhf', # Unrestricted Hartree-Fock to handle open-shell systems  
 'basis': '6-31g', # A reasonable basis set for magnetic behavior  
 'guess': 'sad', # Guess method: Superposition of atomic densities  
 'scf\_type': 'df' # Density fitting to speed up calculations  
})  
  
# Perform a single-point energy calculation  
scf\_energy = psi4.energy('scf')  
  
# Get the wavefunction object to retrieve orbital and spin information  
wfn = psi4.core.Wavefunction.build(molecule, psi4.get\_global\_option('basis'))  
wfn = psi4.energy('scf', return\_wfn=True)[1]  
  
# Calculate the number of unpaired electrons  
alpha\_occ = wfn.nalpha() # Number of alpha electrons (spin-up)  
beta\_occ = wfn.nbeta() # Number of beta electrons (spin-down)  
  
unpaired\_electrons = abs(alpha\_occ - beta\_occ)  
print(f"Number of unpaired electrons: {unpaired\_electrons}")  
  
# Calculate the effective magnetic moment (μ\_eff)  
mu\_eff = np.sqrt(unpaired\_electrons \* (unpaired\_electrons + 2))  
print(f"Effective magnetic moment (μ\_eff): {mu\_eff:.2f} Bohr Magnetons")  
  
# Spin multiplicity calculation  
spin\_multiplicity = unpaired\_electrons + 1  
print(f"Spin multiplicity: {spin\_multiplicity}")  
  
# Additional properties (optional, magnetic susceptibility, dipole moments, etc.)  
# Example: Magnetic susceptibility calculation (χ\_mol)  
psi4.set\_options({'properties': ['magnetic\_susceptibility']})  
properties = psi4.properties('scf')

**Explanation of Code:**

* **Geometry Definition:** The molecule’s geometry is defined using Cartesian coordinates. In the example, we are working with FeCl3\text{FeCl}\_3FeCl3​, but this can be replaced with other compounds such as CoCl2\text{CoCl}\_2CoCl2​, MgO\text{MgO}MgO, or any other molecule you wish to study.
* **Basis Set and SCF Options:** We use the 6-31g basis set, which provides a reasonable level of accuracy. The UHF (Unrestricted Hartree-Fock) method is used to handle open-shell systems, which are typical for paramagnetic compounds with unpaired electrons.
* **Unpaired Electrons Calculation:** The number of unpaired electrons is determined by the difference between the number of alpha and beta electrons in the molecule.
* **Effective Magnetic Moment:** The magnetic moment is calculated using the formula
* **Spin Multiplicity:** The spin multiplicity is calculated as n+1n + 1n+1, where nnn is the number of unpaired electrons. This value is important for interpreting the paramagnetic or diamagnetic nature of the molecule.
* **Question 1:** Based on the Psi4 calculation of the unpaired electrons for FeCl3​, explain whether the compound is paramagnetic or diamagnetic.
* **Question 2:** How does the calculated effective magnetic moment of FeCl3​ compare with the experimental value obtained in the lab? What could account for any differences?
* **Question 3:** Calculate the effective magnetic moment of CoCl2 using Psi4 and compare it with the experimental value you obtained.
* **Question 4:** Explain the relationship between the number of unpaired electrons and the calculated spin multiplicity for FeCl3.
* **Question 5:** How does the basis set and level of theory (e.g., UHF vs. RHF) affect the calculated magnetic properties in Psi4? Could these choices influence the accuracy of your results?

To visualize the magnetic structure of FeCl3​, we need to plot the molecular structure showing the magnetic behavior, such as spin densities or unpaired electrons. We can achieve this by calculating the spin densities using Psi4 and visualizing the molecule in 3D using py3Dmol or matplotlib with additional molecular visualization tools.

The general steps are as follows:

1. **Compute the spin densities using Psi4.**
2. **Extract molecular geometry and spin data.**
3. **Visualize the molecular structure and spin density.**

Below is a Python code that integrates Psi4 for spin density calculations and py3Dmol for 3D visualization of the FeCl3​ molecule. We will focus on plotting the magnetic structure based on unpaired electrons and visualizing the molecule.

**1. Install necessary libraries**

First, install the required libraries:

pip **install** psi4 py3Dmol numpy

2. **Python code for computing and visualizing magnetic structure**

**import** psi4  
**import** py3Dmol  
**import** numpy **as** np  
  
# Set Psi4 memory and output file  
psi4.set\_memory('500 MB')  
psi4.core.set\_output\_file('fecl3\_output.dat', False)  
  
# Define the molecule geometry for FeCl3  
fecl3 = psi4.geometry("""  
Fe 0.0000 0.0000 0.0000  
Cl 1.8000 1.8000 1.8000  
Cl -1.8000 -1.8000 1.8000  
Cl -1.8000 1.8000 -1.8000  
""")  
  
# Set SCF options for UHF (Unrestricted Hartree-Fock) to handle unpaired electrons  
psi4.set\_options({  
 'reference': 'uhf', # Unrestricted Hartree-Fock  
 'basis': '6-31g', # Basis set  
 'guess': 'sad', # Superposition of atomic densities  
 'scf\_type': 'df' # Density fitting for speed  
})  
  
# Perform single-point energy calculation and get wavefunction  
scf\_energy, wfn = psi4.energy('scf', return\_wfn=True)  
  
# Extract spin density  
alpha\_density = wfn.Da().to\_array() # Alpha electron density (spin-up)  
beta\_density = wfn.Db().to\_array() # Beta electron density (spin-down)  
  
# Compute the spin density (difference between alpha and beta)  
spin\_density = alpha\_density - beta\_density  
  
# Get the geometry of the molecule  
geom = wfn.molecule().geometry().to\_array()  
symbols = [wfn.molecule().symbol(i) **for** i **in** range(wfn.molecule().natom())]  
  
# Prepare the molecule for visualization in py3Dmol  
xyz = ""  
**for** i, symbol **in** enumerate(symbols):  
 x, y, z = geom[i]  
 xyz += f"{symbol} {x:.4f} {y:.4f} {z:.4f}\n"  
  
# Visualize the molecule using py3Dmol  
view = py3Dmol.view(width=800, height=600)  
view.addModel(xyz, "xyz")  
view.setStyle({'stick': {}})  
view.addSphere({  
 'center': {'x': 0.0, 'y': 0.0, 'z': 0.0}, # Iron atom at origin  
 'radius': 0.5,  
 'color': 'red' # Indicating Fe atom's contribution to magnetic moment  
})  
  
# Optional: Add spin density visualization (requires a way to render volumetric data)  
# For simplicity, here we show just the molecular structure with magnetic centers highlighted.  
  
# Set the visualization options  
view.zoomTo()  
view.show()

**Explanation of the Code:**

1. **Psi4 Computation:**
   * We define the molecular geometry of FeCl3​ using Cartesian coordinates.
   * The SCF method used is UHF (Unrestricted Hartree-Fock) to handle the open-shell system with unpaired electrons.
   * After performing the SCF calculation, we extract the alpha and beta spin densities to compute the spin density.
2. **Molecular Geometry Extraction:**
   * We retrieve the molecular geometry (position of atoms) and their symbols (Fe, Cl) to prepare the XYZ coordinates for visualization.
3. **3D Visualization with py3Dmol:**
   * The molecular geometry is visualized in 3D using py3Dmol.
   * The central iron atom, which contributes most to the magnetic behavior, is highlighted using a red sphere.
   * This visualization can be enhanced by adding volumetric representations of the spin density (though not implemented in this simple version).

**4. Enhancements:**

* **Spin Density Plot:** You can further enhance the visualization by plotting the spin density around the atoms to better represent the magnetic structure of FeCl3​.
* **Isosurface for Spin Density:** With additional code, you can visualize isosurfaces that represent regions of high spin density around the atoms.

**5. Running the Code:**

When you run the code, a window will open displaying the 3D structure of FeCl3​, with the iron atom at the center highlighted as the main contributor to the magnetic behavior. The script uses UHF to compute the spin density and visualize the molecular structure, aiding in the study of its magnetic properties.

This visualization can be extended to different molecules by simply modifying the molecular geometry section and recalculating using Psi4.

Question 6 Based on the Psi4 output and spin density visualization in the provided code, explain why FeCl3​ is paramagnetic. What role do the unpaired electrons in the iron atom play in this magnetic behavior? How does the molecular structure contribute to this property?

Question 7Modify the code to model and visualize the magnetic structure of cobalt(II) chloride (CoCl2​). Adjust the molecular geometry for CoCl2​ and explain the paramagnetic nature of Co2+ based on its electron configuration. How does the spin density in CoCl2​ compare to that of FeCl3​?

Here's the molecular geometry for CoCl2 to use in your modified code:

Co 0.0000 0.0000 0.0000  
Cl 1.8000 1.8000 1.8000  
Cl -1.8000 -1.8000 -1.8000

Question 8 The current Psi4 calculation for FeCl3​ uses the 6-31G basis set. Experiment with a larger basis set, such as def2-TZVP, and rerun the calculation. Compare the spin density and energy results obtained with the different basis sets. How do these changes affect the accuracy of the magnetic moment calculation and visualization for FeCl3​?

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