ORCA Lab Report

Basis Set Test: HY/PY Tautomers

Due at the end of lab

Student Name: _____

Student ID: _____

Lab Objectives

- Connect to the C1 cluster and set up the ORCA environment
- Build molecular structures for 2-hydroxypyridine (HY) and 2-pyridone (PY)
- Perform geometry optimizations with pc-0
- Compare computational results to experiment

1 System Setup

1.1 Successfully connected to C1 cluster? Yes No

1.2 ORCA path verified with `which orca`? Yes No

1.3 Working directory created: _____

2 Molecular Structures

2.1 Sketch or describe the structural difference between HY and PY:

2.2 Which atoms differ in their bonding between the two tautomers?

3 Computational Results

Complete the following table with your calculated values:

Table 1: Basis Set Convergence Data

Set	$\mathbf{Bond_{OH}}$ (Å)	E(HY) (kJ/mol)	$\mathbf{Bond_{NH}}$ (Å)	E(PY) (kJ/mol)	ΔE (kJ/mol)
pc-0					

*ΔE = E(PY) - E(HY) in kJ/mol. Use conversion: 1 Hartree = 2625.5 kJ/mol

Vibrational Analysis

3.1 Open your `molecule.out` file in Avogadro to visualize the vibrational frequencies.

3.2 What is the highest vibrational mode (frequency in cm^{-1}) for each molecule?

Molecule	Highest Frequency (cm^{-1})
HY	
PY	

3.3 What type of vibration does this highest frequency correspond to? (Hint: Look at the animation in Avogadro)

4 Analysis Questions

4.1 Which tautomer is more stable according to your calculation?

4.2 Literature says that the energy difference between the HY and PY is around -2.4kJ/mol. How does your calculated energy difference compare to the experimental result? Why is there a discrepancy?