

ORCA Lab Report

Basis Set Convergence Study: HY/PY Tautomers

Student Name: _____

Student ID: _____

Lab Section: _____ **Date:** _____

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
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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	Bond _{OH} (Å)	E(HY) (kJ/mol)	Bond _{NH} (Å)	E(PY) (kJ/mol)	ΔE (kJ/mol)
pc-0					

* $\Delta E = E(\text{PY}) - E(\text{HY})$ in kJ/mol. Use conversion: 1 Hartree = 2625.5 kJ/mol

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?

Due at the end of lab