

## ORCA Lab Report

Basis Set Convergence Study: HY/PY Tautomers

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**Student Name:** \_\_\_\_\_

**Student ID:** \_\_\_\_\_

**Lab Section:** \_\_\_\_\_ **Date:** \_\_\_\_\_

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### 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 <sub>OH</sub> (Å)	E(HY) (kJ/mol)	Bond <sub>NH</sub> (Å)	E(PY) (kJ/mol)	ΔE (kJ/mol)
pc-0					

\* $\Delta E = E(PY) - E(HY)$  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?

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**Due at the end of lab**