ORCA Lab Report

Basis Set Convergence Study: HY/PY Tautomers

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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

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: ~/NE-452/DFT/Lab1

2 Molecular Structures

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

The difference between the molecules are that the HY has a Hydroxyl Group where as PY has a Double Bonded Oxygen on the second Carbon. Additionally, HY has a Double Bonded Nitrogen where as PY has a Single Bonded Nitrogen with a Hydrogen on it

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

The Nitrogen and Oxygen differ in their Bonding Between the 2

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	0.989	-846 581.1065	1.027	-846 635.1883	-54.081

*ΔE = 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?

Since Stability in inversely Proportional to Energy, The most Negative is more Stable Meaning 2-Pyridone is more Stable

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?

The result I got was much larger at -54.081 KJ/mol, this is due to the small Basis set used. This shows the importance of Using Better Basis Sets at the cost of Computation Time

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Due at the end of lab

* Note: I Ran Calculations on My own Device Bypassing Slurm. I Hope I don't get Penalized for that