Experiment 6: Lab Report Template

Put Your Name Here

October 6, 2023

Abstract

A good abstract should include a clear statement of the experimental aim, some significant data points presented correctly, as well as a concise summary of trends and observations concerning your data. A great abstract will mention the specific methods used and the validity/level of error in the presnted data. When in doubt, please consult the laboratory report guidelines available on Learn.

1 Introduction

Ideally, your introduction should include a concise summary of the chemistry background for the experiment; an explanation of any key terms and concepts should be given. Aim to include **any and all** information you may need to mount a solid, well-backed discussion section. In-text references and good usage of literature sources are both crucial for a good introduction.

Please make use of relevant figures to illustrate your points. You will also be marked on your use of scientific language and overall presentation. If you aren't sure what is appropriate for academic writing, please consult the many guides available online, such as **this one**.

2 Methodology

Since the energy value is impossible to be measured experimentally, the computational method was used in the experiment to obtain the molecular energy.

Trimethylamine was built via Spartan Student version8. It was optimised using "Equilibrium Geometry" and "Molecular Mechanics" (MMFF). This calculation was repeated using "Semi-Empirical" (PM3) instead of MMFF to obtain more accurate properties about the molecule. The energy and dihedrals of the molecule were recorded. Trimethylamine was constrained to a planar by constraining the dihedral angle to 180 degrees. The planar NH_3 was optimised with the same method. The energy of the planar NH_3 was recorded. These steps were repeated with different molecules: PMe_3, N^iPr_3, P^iPr_3, PBr_3, PCl_3, PF_3, $PPhMe_2$, $PPhMe^tBu$, $P(C_6H_{11})Me^nPr$, $PPhMe^nPr$, $PPhMe(4-MePh)$, $PPhMe(SiH_3)$, PPh^iPr^tBu, PPh^iPr^tBu, $(H_2CCH_2)NMe$.

Triplet carbene ligand (-C(OMe)Me) was built and optimised using MMFF first followed by PM3 method with "Equilibrium Geometry". This step was repeated with Singlet (-C(OMe)Me), Triplet ($-CH_2$), Singlet($-CH_2$). The energy of triplet states and Singlet states for each carbene ligand were compared to determine the ground electronic state of Fischer (-C(OMe)Me) and Schrock ($-CH_2$) structure. The molecular orbitals of -C(OMe)Me and $-CH_2$ were obtained, and the energy of the σ-donating and π-accepting orbitals were recorded.

Four different structures of $Ph(OMe)CCr(CO)_5$ - (syn, eclipsed), (syn, staggered), (anti, eclipsed), and (anti, stagered) - were built and optimised. Their energy were compared to determine the stablest structure. The C-O bond distance and the electrostatic of the central carbon were recorded.

$Ph(NH_2)CCr(CO)_5$, $TaCp_2Me(CH_2)$, and $TaCp_2Me(CH_2)AlMe_3$ were built and optimised using the same method. The electrostatic of the central carbon for each molecule was recorded.

3 Results

The ground state energy, the energy after constrained to a planar, and the dihedral angles of NMe_3, PMe_3, N^iPr_3, P^iPr_3, PBr_3, PCl_3, PF_3, $PPhMe_2$, $PPhMe^tBu$, $P(C_6H_{11})Me^nPr$, $PPhMe^nPr$, $PPhMe(4-MePh)$, $PPhMe(SiH_3)$, PPh^iPr^tBu, PPh^iPr^tBu, $(H_2CCH_2)NMe$ were recorded in Table 1. The activation energy of inversion for a molecule is calculated by subtracting the ground state energy from the energy of planar, and the result was recorded in Table 1.

The energy of Fischer (-C(OMe)Me) and Schrock ($-CH_2$) in both Triplet states and Singlet states were recorded in Table 2.

The σ-donating and π-accepting orbital of Fishcer (-C(OMe)Me) and Schrock ($-CH_2$) carbene ligand were shown in Figure 1. The energy of the HOMO for -C(OMe)Me was -9.1 eV and LUMO was 0.5 eV. The energy

Table 1: *Energy of each molecule in the ground state (E), and the energy of the molecule when it constrained to a planar (E') were recorded. The activation energy of inversion (E_a).*

Name of the Molecules	E (kJ/mol)	E' (kJ/mol)	E_a (kJ/mol)
Line 1	68.28	45.30	56.79
Line 1	68.28	45.30	56.79
Line 1	68.28	45.30	56.79
Line 1	68.28	45.30	56.79
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Line 1	68.28	45.30	56.79
Line 1	68.28	45.30	56.79
Line 1	68.28	45.30	56.79
Line 2	54.06	38.63	46.35
Line 3	61.17	41.97	

Table 2: *The energy of Fischer and Schrock carbene ligand in triplet and singlet state.*

Name of the molecules	E (Triplet) (kJ/mol)	E (Singlet) (kJ/mol)
-C(OMe)Me	51.41	14.56
-CH2	299.72	473.74

of HOMO for -CH_2 is -10.4eV and HOMO-1 was 11.5 eV.

C(OMe)Me HOMO white background.png

Figure 1: *Same*

The energy and C-O bond length of $Ph(OMe)CCr(CO)_5$ in four different structures were recorded in Table 3. The syn-conformation had lower energy than the anti-conformation, and the eclipsed form had lower energy than the staggered form. The syn-eclipsed structure had the lowest energy, meaning that the molecule was most stable under this structure.

Table 3: *The energy of $Ph(OMe)CCr(CO)_5$ in four different structures*

Conformation	Syn	Anti
Eclipsed	-774.75 kJ/mol	-751.85 kJ/mol
Staggered	-772.83 kJ/mol	-755.68 kJ/mol

The charge of the central carbon of $Ph(OMe)CCr(CO)_5$, $Ph(NH_2)CCr(CO)_5$, $TaCp_2Me(CH_2)$, and $TaCp_2Me(CH_2)AlMe_3$ were recorded in Table 4. For Fischer carbene (-C(OMe)Me) molecule, the charge of the central carbon was less positive as the -OMe group was replaced by -NH_2 group, meaning it is less electrophilic. For Schrock (-CH_2) carbene, the charge of the central carbon become less negative, which indicates that the carbon become less nucleophilic when $AlMe_3$ was added to the central carbon.

Table 4: *The charge of the central carbon of Fischer and Schrock carbenes*

Name of the molecules	electrostatic (eV)
$Ph(OMe)CCr(CO)_5$	
$Ph(NH_2)CCr(CO)_5$	
$TaCp_2Me(CH_2)$	
$TaCp_2Me(CH_2)AlMe_3$	

Please make sure you describe the data, particularly any trends that are apparent – always avoid data-dumps. The best result section will guide the reader through the data, pointing out any important trends, values, or possible errors.

If you wish to learn more about how to format tables, please visit **this page**. You can also find a handy tool which can generate tables for you here: https://www.tablesgenerator.com/

4 Discussion

Part 1

The activation energy needed for inversion varies among different molecules.

1. Nature of the central atom

N^iPr_3 vs. P^iPr_3

2. Substituent Effect
PBr_3 vs. PF_3 vs. PCl_3

3. Steric effect
$PPhMe_2$ vs. $PPhMe^tBu$

4. Conjugation effects
$P(C_6H_11)Me^nPr$ vs. $PPhMe^nPr$

5. Ring strain effects

Part 2

The energy of a triplet Fischer ligand ($C(OMe)Me$) was higher than the energy of its singlet form as shown in **Table x**, meaning that it was more stable for a Fischer molecule to stay in a singlet form. Thus, the ground electronic state of Fischer ligands were singlet states instead of triplet states. However, for a Schrock ligand (CH_2), the energy of its triplet state was lower than its singlet states, meaning that triplet states is more stable for Schrock ligands. Therefore, the ground electronic state of Schrock ligands is triplet states. The molecular orbital diagram of both CH_2 and $C(OMe)Me$ were shown in the **Figure x**. As CH_2 was a triplet, the energy of the two highest occupied molecular orbitals (HOMO) were very close, so the stablest structures

This again compares well with the experimental crystal structure of [Cr(CO)5(C(OMe)Ph)], which adopts this same geometry.

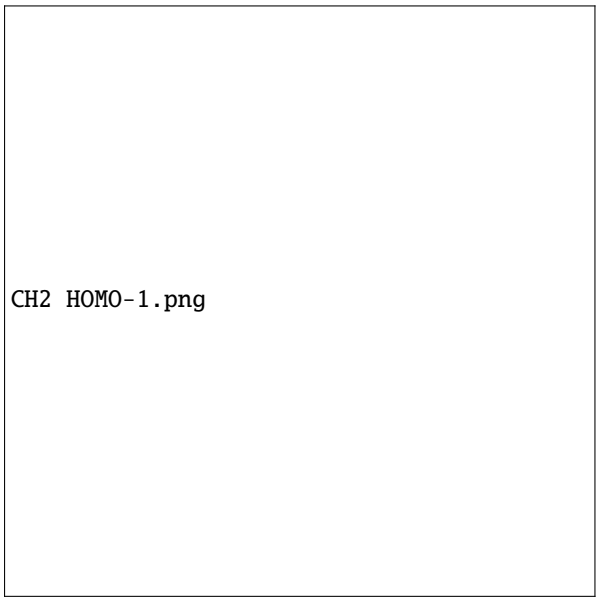

Figure 2: *Same*

Make use of figures and/or external references to support your discussion points. An example figure is shown above as Figure 1.

The best discussion will also include a brief paragraph with conclusions (for each part of the experiment) and future work. Future work, in this case, refers to a brief discussion on the validity of your chosen method, and the justification of using computational methods for the purposes of this experiment. The best discussion will offer some suggestions on the improvement of the experimental design.

Please use concise and scientific tone in your writing. Academic writing, by convention, uses the past tense and a passive voice. Try to emulate the style you see in textbooks/papers. Avoid the use of first (I/we) or second (you) person, informal language, overuse of conjunctions and pronouns (especially 'this/that'). Make sure to proofread and spellcheck your work before submitting!

Again, if you aren't sure what is appropriate for academic writing, please consult the many guides available online, such as **this one**

5 Investigation Question

Please include the write-up to your investigation question here. Include any relevant figures, sources, or background information, as instructed in your manual.
The best Investigation Question will include:
1) a short, relevant introduction to the problem,
2) a clear and well-worded proposal of a solution (hypothesis), and
3) a concise and well-researched backing/explanation for the solution.

Use appropriate scientific language and make sure to properly reference all of your sources!

Note on the Citation

All sources should be formatted in the Royal Society of Chemistry (RSC) referencing style[?] . If you don't know what this means, I strongly recommend reviewing how citation and referencing works in general, and looking into the style guides for the RSC style in particular.

If you use a different referencing style (MLA, Harward, etc.) please indicate so in a footnote[i] of your citation section, so that the demonstrator marking your work knows that you've used something different and can check it for errors!

With Overleaf, you can simply import a .bib file into your file tree (the panel on the left-most side of your screen) and the bibliography command will automatically compile them for you. Please make sure to include relevant in-text references using the \cite command. The \printbibliography

[i] Example on how to format a footnote in LaTeX

command will then generate the proper references section for you!

.bib file can be easily obtained using a reference-management software. If you don't know what this is, or don't yet use one, I **strongly** recommend looking into one! Personally, I use Mendeley, which has both a desktop version and a browser plug-in — this enables you to add references as you browse/research. If you learn how to use a reference management software now, it will save you tons of time later on; while you're writing your thesis, or other works in the future.

Further guidelines on referencing in LaTeX can be found here: https://www.overleaf.com/learn/latex/Bibliography_management_in_LaTeX

Tips and Tricks

LaTeX is a widely used compiler, there are hundreds of tutorial articles and videos online - please make use of them! Google is your friend, you need only ask.

How to write Mathematics

LaTeX is great at typesetting mathematics. Let $X_1, X_2, \ldots, X_n$ be a sequence of independent and identically distributed random variables with $\mathrm{E}[X_i] = \mu$ and $\mathrm{Var}[X_i] = \sigma^2 < \infty$, and let

$$S_n = \frac{X_1 + X_2 + \cdots + X_n}{n} = \frac{1}{n} \sum_{i}^{n} X_i$$

denote their mean. Then as n approaches infinity, the random variables $\sqrt{n}(S_n - \mu)$ converge in distribution to a normal $\mathcal{N}(0, \sigma^2)$.

How to add Lists

You can make lists with automatic numbering . . .

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