**5 Pros and Cons**

Pros:

1. The Clean in 2D function was really helpful and helped me see the structures better.
2. The function of dragging selected structures made formatting easier.
3. The function of “Structure to Name” helped me check the IUPAC name.
4. The Insert Object function helped me add and format the text needed, making it easier to just put the molecules on one page, instead of putting the images directly on word.
5. The Table of Radicals helped me save time by not making me have draw my own benzene rings.

Cons

1. Deciding how to start with the molecules was a bit difficult.
2. Initially putting the chemicals in word, it was hard to find a way to format all the molecules easily, until I finally stumbled upon the Insert Object function stated before.
3. I struggled to form a few of the structures because I did not keep in mind the rules of chemistry.
4. I struggled with making new bonds because I was not attaching the bond to the center atom.
5. Some of the structures had letter combinations that I was not sure of, so an explanation how to proceed with those would be helpful.

**Part 3 – SciFinder Scholar**

CAS: 100-39-0 CAS: 637-59-2 CAS: 705-29-3

Diagram

Description automatically generated

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Course 3111 Section 12

Dr. Zhifo Guo

Time and Effort Assessment

This was not a conventional lab. I did enjoy that we got to do this on our own and on our own time, though it did take much longer than expected. While initially beginning this lab, it took much effort to access the right websites and get all the programs downloaded and opened correctly. When I had finally accessed the right resources, I was able to pick an article relatively quickly. The second hardest part of this lab came when I decided to take screenshots of the molecules I had made on ChemSketch. I later discovered it was easier to make and format items on ChemSketch, and then just convert it into a pdf. Avogadro was not much of a challenge as it was self-explanatory. It was, however, very tiresome, as I had forgotten to turn off the “Auto Optimization Tool” before adding to the molecules, making the whole molecule shift more and the stabilization take longer than needed. Overall, I am glad we got 2 weeks to work on this lab as it was very necessary, especially with the midterms that we had to take.

JOC Reference:

*Journal of Organic Chemistry, Volume 67, No. 1, 2002*

**Part 4 – Theoretical Calculations using Avogadro**

Part A.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Groups** | | **Gauche** | | **Anti** | |  | (Opt. Gauche Angle) – (60­­O) | (Gauche E) – (Anti E)  (kJ/mol) |
| **R1** | **R2** | **Opt. Angle** | **E (kJ/mol)** | **Opt. Angle** | **E (kJ/mol)** |  |
| Me | Me | 64.4­­O | ­­14.06 | 180­­O | 7.423 |  | 4.4­­O | 6.637 |
| Me | tBu | 68.6­­O | 78.086 | 180­­O | 42.985 |  | 8.6­­O | 35.101 |
| tBu | tBu | 99.3­­O | 167.025 | 180­­O | 79.237 |  | 39.9­­O | 87.788 |

As we go down the column, it is clear that the gauche optimum angle increases. This initially does not make sense, as the largest angle 6 molecule could have from each other would be 60­­O. However, if we look at the R1 and R2, we notice that the groups slowly grow larger. As the groups keep growing, they will “push” more to get farther away. Beyond this, the largest groups will want to be the farthest apart as possible, so the largest angles still considered to have a gauche interaction would be caused by the groups attached to the central carbons. It is important to note that these groups should not be eclipsed due to the hydrogens connected to the central two carbons.

When comparing the gauche and anti steric energies, we can see that the anti conformations naturally had lower values. Steric energy is dependent on the strength of two groups which may be close enough to cause an overlap of large electron clouds. Steric energy increases as carbon substitution does, which is primary < secondary < tertiary < quaternary carbons. As carbon substitution increases, the electron clouds will overlap more, thereby increasing the steric strain. The best way to reduce steric strain is by allowing the large groups to be as far away from each other as possible, a position also known as anti. Sometimes, the electron clouds will form a gauche interaction with the ring. Gauche interactions increase as the strength of the interactions between the electron clouds increase. Conceptually, the anti conformations should have lower steric energies, as the largest groups should be the farthest apart from each other. This is true for both homo interactions, involving the same group, or with hetero interactions, involving different groups. The only difference between the interactions is that the different groups will push differently, so the larger groups would contribute more to the steric energy, rather than the smaller (but still important) group. These trends are easily applicable and are evident in the chart above.

Part B.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **R3** | **Axial (kJ/mol)** | **Equatorial (kJ/mol)** | **Axial (kcal/mol)** | **Equatorial (kcal/mol)** | **Calculated A-Value (kcal/mol)** | **Literature A-Value (kcal/mol)** | **Difference** |
| Me | 49.088 | 34.998 | 11.732 | 8.365 | 8.365 | 1.7 | 6.665 |
| tBu | 155.897 | 90.202 | 37.26 | 21.559 | 21.559 | 5.4 | 16.159 |
| Br | 38.481 | 26.541 | 9.197 | 6.343 | 6.343 | 0.6 | 6.283 |

As shown by the last column, there was a large difference between the literature (experimental) value and the calculated (theoretical) values. Considering that we used a simple program, a little difference between the theoretical and experimental values is to be expected, but I would consider my calculated difference quite catastrophic. It can be theorized that under certain circumstances, my values could be valid, as these results depend on experimental conditions and setups that, if differed in the slightest way, can change the result. However, the general trend for my A-values followed that of the literature A-values, in that the A-value increased from Br < Me < tBu, as larger carbon substitutions took place. It is safe to conclude that though online tools are convenient and popular, they may not be as accurate as needed.