Reaction Coordinate in ADF
Project (200 Points)

CHEM 4631/5631, Spring 2022
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1 Project Overview

Using ADF, you will create a reaction coordinate for a one-step (or one-step of a) chemical reaction of your choice. This involves determining the transition state for the reaction and performing and intrinsic reaction coordinate (IRC) calculation. You will also analyze the bonding interactions in the reactants and products using a variety of methods.

Your results will be presented in the form of both a journal article and presentation to the class.

2 Required Calculations

The following are the minimum requirements for this project, which will results in a C grade (75%) if performed adequately.

2.1 Reaction model

- Create a reaction coordinate for a one-step (or one-step of a) reaction in the gas phase.
  - Find a transition state (TS) structure by performing a TS search and verify this structure with a frequency calculation
  - Perform an intrinsic reaction coordinate (IRC) to create a full reaction coordinate
  - Verify your reactant and product states with a frequency calculation
- Justify your choice of basis set and functional for your calculations based on other literature.

2.2 Analysis of results

- Analyze how the geometry of your molecule(s) change from reactant $\longrightarrow$ TS $\longrightarrow$ product
- Calculate the rate of the forward and reverse reactions

3 Optional Calculations

You may choose from the following optional calculations to improve your overall project grade from a C to a B or A grade. If you perform one additional reaction calculation or analysis method you

will be eligible for a B grade. If you perform at least two additional reaction calculations or analysis methods you will be eligible for an A grade. You may also perform calculations not listed below, with instructor approval.

3.1 Reaction model

- If you chose a multi-step reaction, create a reaction coordinate (using the same procedure in the required reaction model calculations) for another step in your reaction.
- If your chosen reaction occurs in solution, create a second reaction coordinate (of the same step you used for the required reaction model calculation) that includes solvation. Compare this to your gas-phase reaction coordinate.
- If your chosen reaction can be performed with a catalyst, create a second reaction coordinate (of the same step you used for the required reaction model calculation) that shows this alternative reaction pathway.

3.2 Analysis of results Each of the analysis options below includes a hyperlink to an ADF tutorial showing you how the analysis method works.

- Fragment analysis: `https://www.scm.com/doc/Tutorials/Analysis/FragmentAnalysis.html#fragment`
- QTAIM analysis: `https://www.scm.com/doc/Tutorials/Analysis/QTAIM.html#qtaim`
- EDA analysis: `https://www.scm.com/doc/Tutorials/Analysis/EDA.html#eda-adf`
- Visualization of densities and other properties: `https://www.scm.com/doc/Tutorials/Analysis/VisualizationOfDensitiesEtc.html#advancedamsview`
- Fukui functions: `https://www.scm.com/doc/Tutorials/Analysis/FukuiFunctionsAndDualDescriptor.html#fukui`
- Any other analysis method that makes sense for your chosen reaction such as determining spectra, analyzing molecular orbitals, etc.

4 Journal Article

This project will be reported as if you were going to submit this as an article in the Journal of the American Chemical Society (JACS). You are encouraged to visit the ACS web page for further information about submission of a full article manuscript and to find an article template for Microsoft Word or LaTex. The report will consist of a title, abstract, introduction, methods, results/discussion, conclusion, and references. All citations, figures, and tables, will comply with the regulations set forth by the ACS (this includes but is not limited to the resolution of the figures, and the format of the citations). You are encouraged to use a reference package such as Mendely, Zoltero, RefWorks, or BibDesk to organize your citations.

Consider the following when writing your journal article:

- Perform a search to find relevant literature that supports your hypothesis, methods, and importance of the current research

- Abstract: the abstract should succinctly outline the work conducted and highlight the most important discoveries.
- Introduction: the introduction should set the stage for the reported research. Enough information should be presented to show competence in the chemical system being modeled and the use of DFT methods, citing the pertinent articles in the literature.
- Methods: clearly outline the methodology used in the analysis. You do not have to include a section describing all the gory details of the quantum mechanical methods. Look at the relevant literature and see what a typical methods section for calculations entails. Generally, you will see the Schrödinger equation or basic DFT equations, a few lines indicating and justifying the level of theory used, a few lines indicating and justifying the basis set used, and a small section on the calculations/analyses performed.
- Results/Discussion: ability to use the concepts taught in this class and other literature to analyze the data. Be creative and use multiple analysis methods when possible to collect and analyze your results
- Conclusion: ability to concisely write a conclusion that highlights the important discoveries and their relevance to science and/or society. The conclusion section should be at a minimum a small paragraph (at least 4 lines).
- Figures & tables: these should be clearly readable and convey as much pertinent information as possible
- References: you should have at least 10 references and at least 2 of these references should be related to the methods you are using to run your calculations and/or analyze your results

5 Presentation

Each student will give an 8-12 minute presentation on their project followed by approximately 5 minutes for questions. A general guideline for your presentation format is that you should include 1-2 slides of background information on the chosen reaction, 2-4 slides on the specific methods utilized, 2-4 slides of results, and 1 slide for conclusions. The exact number of slides will vary for each project.

6 Grading Rubric

Item	**Points**
Approval for chosen reaction	10
Journal article	100 total
Title	5
Abstract	10
Introduction	15
Methods	20
Results/Discussion	25
Conclusion	10
References	5
Formatting/Spelling/Grammer	10
Presentation	40 total
Background information	5
Methods	10
Results	10
Time management	5
Clarity	5
Q & A	5
1st calculation beyond minimum requirements	25
2nd calculation beyond minimum requirements	25
Total	**200**