

General outline for an “ideal” heat of combustion lab report

Results

- Refer reader to data tables containing computational results; two tables should be included
 - Table of geometries, vibrations for CO₂, H₂O and O₂
 - Table of calculated enthalpies
- Discuss the set up of the tables and what is included in each
- Generally discuss computational results (pick out highlights); things which *could be* included
 - What had the highest and/or lowest heat of combustion?
 - How were experimental heats of combustion calculated, and what literature values were used?
 - How did AM1 compare to PM3; how did each compare to the experimental data?
 - Were there any anomalies or outliers?
 - Are there any potential sources of error known?
 - Do all calculations on the same molecule agree? If not, did you calculate averages?
- Refer reader to the experimental vs. computational heats graph
 - Explain set up of the graph
 - Give the linear regression info, including the equation (not just R², which by itself is not all that meaningful...)

Discussion

- Address bullet points from the lab
 - Compare the accuracy of your calculations—does one method seem to be better? How do you know (esp. what is the meaning of the regression slope)? Does there appear to be a systematic error in one/both methods? What might the source of such an error be?
 - What is the best fuel *based on the calculations*? Which is most efficient? Is there a noticeable trend in what makes a good fuel (e.g. presence/lack of oxygen, large/small molecules, saturated/unsaturated hydrocarbons, etc.)?
 - Compare ethanol, E85 and E10 as fuels
- Are there any other trends you observed? (i.e., relationships between heats of combustion and molecular structure)
- Were the objectives of the experiment met/achieved?
- Are there things which could have been done differently?
- Were there other calculations which might have made interpreting your data easier?