MM Molecular Modeling Project as of 1/14/08 info may be added

Project and paper format

Select article from set of articles provided in lab and return papers to Rybolt. At end of lab give me piece of paper with your names and letter of paper selected and discuss what you have done that day. Plan, carry out a well done computational project, and write paper using outline given below. Label sections of you report based on outline below. You will have MM periods in lab to work on project but may also need additional time.

Title page

--title of your paper, author's names, and date work completed

Abstract page

--state problem, approach used, and key results in 200 words or less

1. Introduction

--background, what others have done, detailed explanation of computational method used, and objective of this work

2. Computational Method

--explain theory of method used and what you did

3. Results

--what values were obtained and so most tables and figures in this section

--present and compare prior experimental results, prior calculated results, and your calculated results

4. Discussion

--comparison of your results to earlier work and significance of your results

5. Conclusion

--brief summary of what was done and future work that could be done

6. References

--list references (all sources that you used)

On due dates for each MM period you need to turn in:

MM_1 your paper title and brief description of your plan

MM_2 Title page and section 1. Introduction

MM_3 final paper (one printed copy and a Microsoft Word Document sent to me as attachment)

Computational methods that can be used (discuss with me)

Mechanics	MM2 MM3 etc
Semi-empirical	AM1 PM3 PM5 etc.
Density functional theory	DFT----
Ab initio Hartree Fock	Gaussian---

CAChe software does top three. CAChe with Gaussian03 on one computer (back corner and marked with card) does ab initio but be prepared for long run times (may need to run overnight if big molecule) Always do MM before more complicated methods.