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DEPARTMENT OF CHEMISTRY

BOND-BASED CORRECTIONS TO IMPROVE ATOMIZATION ENERGY  
CALCULATIONS

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## ABSTRACT

In this thesis, we report on a technique to improve atomization energy calculations by various computational methods. Specifically, we have formulated a list of bond-based correction factors that are optimized to improve an inaccurate and computationally inexpensive calculation to yield a result that matches a more accurate but expensive calculation. A summary of our tests is listed below:

Table: List of tests performed in this project.

Test #	# Molecules	Inexpensive Calculation		Expensive Calculation	
		Computational Method	Basis Set	Computational Method	Basis Set
1	71	MP2	6-31G*	MP4	6-31G*
2	71	MP2	6-31G*	MP4	6-311G**
3	25	MP2	STO-3G	MP4	STO-3G
4	25	MP2	6-31G*	MP4	6-31G*
5	25	MP2	6-311G*	MP4	6-311G*
6	24	MP2	STO-3G	MP4	6-311+G(2d,p)
7	24	MP2	6-31G*	MP4	6-311+G(2d,p)
8	24	MP2	6-311G*	MP4	6-311+G(2d,p)

We compared the root mean square (rms) error for corrected and uncorrected atomization energies as the tool to determine the success of the bond-based correction factors. Our results showed that the correction factors significantly improved the inaccurate computational methods, improving the rms error by as much as two orders of magnitude. Results from our experiment can be applied to any molecule with C, H, and O atoms. In the future, it would be useful to add the nitrogen atom to our study, which would make our results applicable to a wider range of molecules.

Finally, it would be interesting to study the usefulness of bond-based corrections as computational methods become more accurate. We speculate that such corrections would become even more effective as computational methods are improved.

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## CHAPTER 1 INTRODUCTION

The field of computational chemistry uses theoretical chemistry, incorporated with computer programs, to assist in solving chemical problems. Because the quantum body problem can be solved analytically only for hydrogen-like systems, it becomes useful to use computers to help solve tedious approximations. Computational methods are used to predict or confirm a wide variety of properties of chemical systems. Examples of such properties include electronic structure, energies, charge distribution, and vibrational frequencies. More novel calculations can predict NMR and IR spectra and reaction mechanisms.<sup>1</sup>

Presently, there exist many computational methods including *ab initio* methods such as Hartree-Fock and Moller-Plesset perturbation theory, density functional methods, and semi-empirical methods such as AM1 and PM3. *Ab initio* - literally meaning “from the beginning” – computational methods are performed primarily using only theoretical principles, without experimental data. The advantage of *ab initio* calculations is that they can converge into exact solutions if all approximations are removed or made sufficiently small. Of course the disadvantage of *ab initio* methods is their computation cost, requiring significant computation time, memory, and disk space.

Density Functional Theory has been developed for large systems. Its advantage is that the theory is based on electron density instead of wave functions, which significantly reduces computational time. As such, there has been a rapid increase in the development of density functional theory to perform calculations on proteins, metals and semiconductors. For example, Zhao *et al.*<sup>2</sup> demonstrated the effects of gas molecules on the electronic and transport properties of single-walled carbon nanotubes using density functional theory. Indeed, DFT holds

tremendous promise for the development of both inorganic materials and biologically useful compounds.

Semi-empirical methods, although based on *ab initio*, make approximations based on empirical data. Semi-empirical calculations are also inexpensive in terms of computation cost. However, results can be erratic if the molecule being computed is not similar enough to the molecules used for approximations in the method. Semi-empirical methods have been extremely useful for organic compounds where only a few elements are used and functional groups recur through different compounds.<sup>3</sup>

Regardless of computational method, however, there is a trade-off between accuracy of calculation and computational cost.<sup>4</sup> This can be illustrated by the Moller-Plesset perturbation theory, which improves upon the Hartree-Fock method by incorporating electron correlation by using the Rayleigh-Schrodinger perturbation theory to the second, third, or fourth order. A fourth order calculation (MP4), although more accurate, takes significantly longer than a third order (MP3). In the same manner, an MP3 calculation is more accurate and time consuming than an MP2 calculation.<sup>5</sup>

During a calculation, in addition to computational method, a chemist generally has to choose a basis set, which are approximations of atomic orbitals. Similarly to computational method, there is a trade-off between accuracy and cost. Smaller basis sets such as 6-31G\* are quick but inaccurate, while larger, complex basis sets such as 6-311+G(2d,p) are more accurate but require longer computing time. It easily becomes evident that one of the largest roadblocks in the field of computational chemistry is the time cost of accurate calculations.

There is considerable amount of research in the field of computational chemistry that focuses on reducing computing cost of various computational methods.<sup>6,7,8</sup>

In this paper, we discuss a simple technique to address this issue: formulating a list of bond-based correction factors that are optimized to improve a “cheap” computational method to yield a result that matches more accurate and expensive calculation. We hypothesize that we can improve the accuracy of several types of computational methods with such correction factors.

## CHAPTER 2 METHODS

The scope of this project was limited to improving the accuracy of atomization energies of molecules with C, H, and O atoms. Atomization energy was calculated by first calculating total energy of a molecule and then subtracting the energy of each of its atoms, using the same computational method and basis set.

The corrected atomization energy,  $\Delta E_{\text{corr}}$ , will be expressed as the sum of the cheaply calculated atomization energy,  $\Delta E_{\text{calc}}$  and a set of correction values,  $c_j$ , for each type of bond  $j$  present in the species. A set of 7 bonds was used for corrections (C-H, C-C, C=C, C $\equiv$ C, C-O, C=O, O-H) and a correction factor for each bond was developed in every test.

We used Monte Carlo methods and FORTRAN programming to develop correction factors that minimized deviations of  $\Delta E_{\text{corr}}$  from the expensive calculations.



CHAPTER 3  
RESULTS PART 1: INITIAL TESTS

The first experiment was designed to determine the validity of correction factors. We chose 71 molecules that included various types of organic functional groups as well as different types of inorganic compounds. We designed an experiment (see Table 1) utilizing popular computational methods and basis sets on the Computational Chemistry Comparison and Benchmark Database by the National Institute of Standards and Technology (NIST). The first test improved an MP2 calculation to MP3 both using the 6-31G\* basis set. The second test improved an MP2 calculation from the 6-31G\* basis set to 6-311G\*\* basis set.

Table 1: Summary of Tests 1 and 2 performed in Experiment 1.

Test #	Inexpensive Calculation		Improve to:	Expensive Calculation	
	Computational Method	Basis Set	Computational Method	Basis Set	
1	MP2	6-31G*	MP3	6-31G*	
2	MP2	6-31G*	MP2	6-311G**	

The root mean square errors for corrected and uncorrected atomization energies for both tests are shown in Table 2 and the correction factors are listed in Table 3.

Table 2: Rms error in atomization energy for Tests 1 and 2.

Correction Type	Rms error in Atomization Energy (hartrees)	
	<i>Uncorrected</i>	<i>Corrected</i>
MP2, 6-31G* → MP3, 6-31G*	0.029342	0.002713
MP2, 6-31G* → MP2, 6-311G**	0.055942	0.001020

As seen in Table 2, the correction factors listed in Table 3 vastly improved the rms error for both tests. For both tests, the rms error was reduced by approximately one order of magnitude.

Table 3: Bond-based corrections developed in Tests 1 and 2.

Bond Type	Correction Factors (hartrees)	
	<i>MP2, 6-31G* → MP3, 6-31G*</i>	<i>MP2, 6-31G* → MP2, 6-311G**</i>
C-C	0.003791194	0.000486988
C-H	$8.86346 \cdot 10^{-6}$	-0.007296489
C=C	0.009246453	0.000437673
C-O	0.00973226	0.00156959
C=O	0.02491584	0.00072159
O-H	0.0026417	-0.0136145
C≡C	0.0185751	-0.0007018

To further analyze results, we plotted “predicted” versus “actual” atomization energies for each test, shown in Figures 1 and 2. Here, “actual” represents the more accurate calculation while “predicted” represents the inaccurate calculation with added correction factors. In these graphs, the slope of the linear equation represents the success of the correction factors in improving the inaccurate calculation. A slope of 1 would show perfect corrections.

As seen in Figures 1 and 2, the slopes were 0.9995 and 1.000 for Test 1 and Test 2, respectively. Indeed, this shows the success of the correction factors in improving atomization energies. Furthermore, the  $R^2$  value of both lines was 1.0000, giving us confidence in the linear fit.

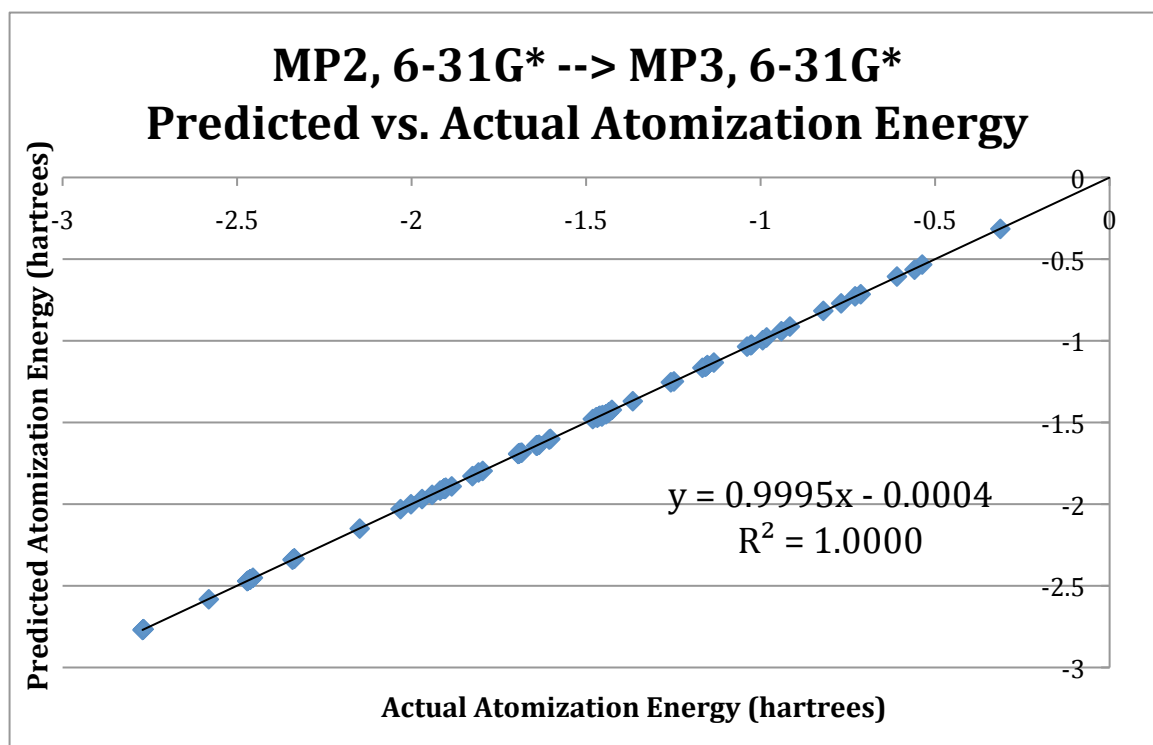


Figure 1: Predicted vs. actual atomization energies for Test 1, in which we corrected from MP2/6-31G\* to MP3/6-31G\*.

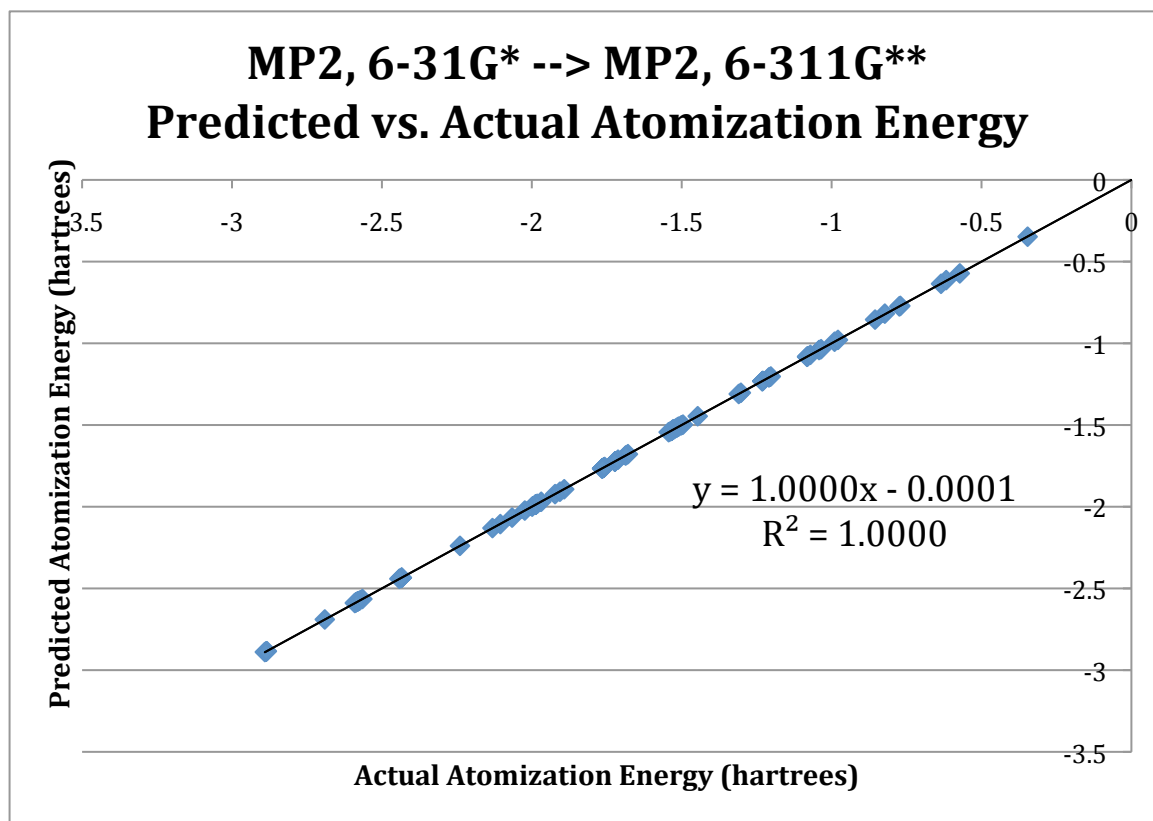


Figure 2: Predicted vs. actual atomization energies for Test 2, in which we corrected from MP2/6-31G\* to MP2/6-311G\*\*.

CHAPTER 4  
RESULTS PART 2: CORRECTIONS FROM MP2 TO MP4

After promising results from the first experiment, we designed another experiment in which we held the computational methods constant while improving the basis set. For each of the three tests, we improved from an MP2 to MP4 calculation and varied basis sets: STO-3G, 6-31G\*, and 6-311G\* (see Table 4).

Table 4: Summary of Tests 3, 4, and 5 performed in Experiment 2.

Test #	Inexpensive Calculation		Improve to:	Expensive Calculation	
	Computational Method	Basis Set	Computational Method	Basis Set	
3	MP2	STO-3G	MP4	STO-3G	
4	MP2	6-31G*	MP4	6-31G*	
5	MP2	6-311G*	MP4	6-311G*	

The rms errors for both corrected and uncorrected atomization energies are listed in Table 5. Table 6 lists the correction factors for each type of bond that were developed in this test.

Table 5: Rms error in atomization energies for Tests 3, 4, and 5.

Correction Type	Rms error in Atomization Energy (hartrees)	
	<i>Uncorrected</i>	<i>Corrected</i>
MP2, STO-3G → MP4, STO-3G	0.0300197	0.00747527
MP2, 6-31G* → MP4, 6-31G*	0.0130180	0.00429517
MP2, 6-311G* → MP4, 6-311G*	0.0300197	0.00066826

As evident from Table 5, the correction factors significantly improved the rms error for each test. For both the STO-3G and 6-31G\* basis sets, the rms error improved by one order of magnitude. For the 6-311G\* basis set, the correction factors improved the rms error by two orders of magnitude.

Table 6: Bond-based correction factors developed in Tests 3, 4, and 5.

Bond Type	Correction Factors (hartrees)		
	<i>MP2, STO-3G</i> → <i>MP4, STO-3G</i>	<i>MP2, 6-31G*</i> → <i>MP4, 6-31G*</i>	<i>MP2, 6-311G*</i> → <i>MP4, 6-311G*</i>
C-C	-0.001544799	0.002868558	0.005515511
C-H	-0.002968356	-0.000460745	-0.001357408
C=C	-0.004435307	0.004143983	0.007911915
C-O	0.004095101	0.005684947	0.006619361
C=O	-0.008591344	0.011600746	0.011041379
O-H	-0.010457246	0.00248455	0.001723713
C≡C	0.008524566	0.009120471	0.013711804

We again plotted predicted vs. actual atomization energies for each test. As seen in Figures 3, 4, and 5, the slopes were 1.0012, 0.9975, and 0.9997 for Tests 3, 4, and 5 respectively. Furthermore, the  $R^2$  values ranged from 0.9998, 0.9999, and 1.000, respectively - once again giving us confidence of the good fit of the regression line.

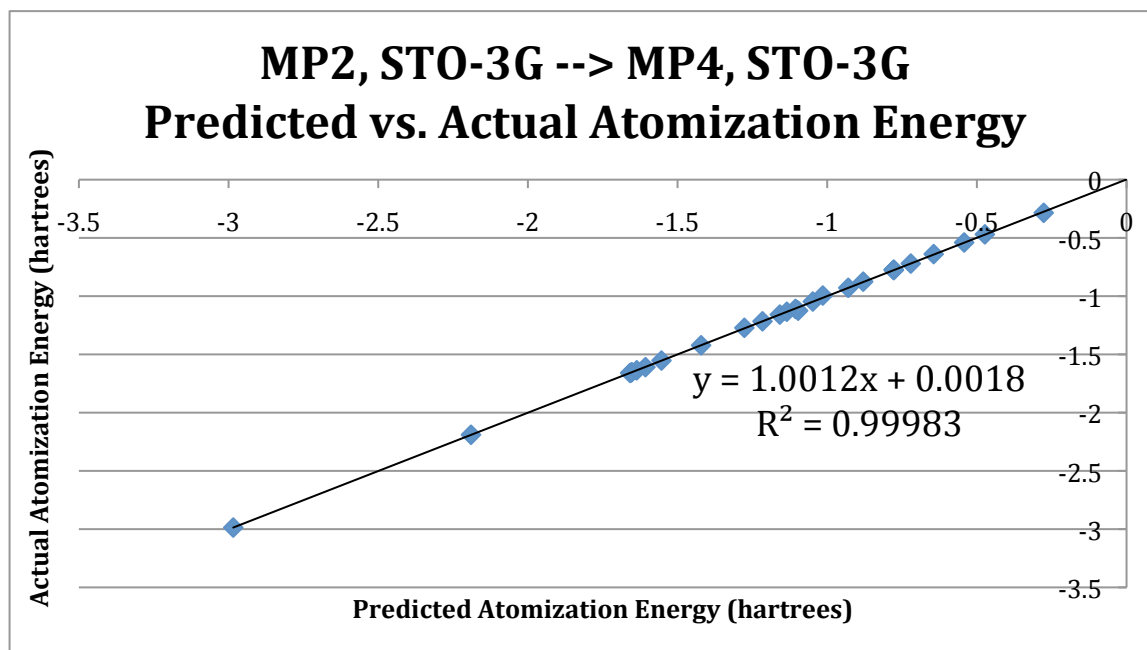


Figure 3: Predicted vs. actual atomization energies for Test 3, in which we corrected from MP2/STO-3G to MP4/STO-3G

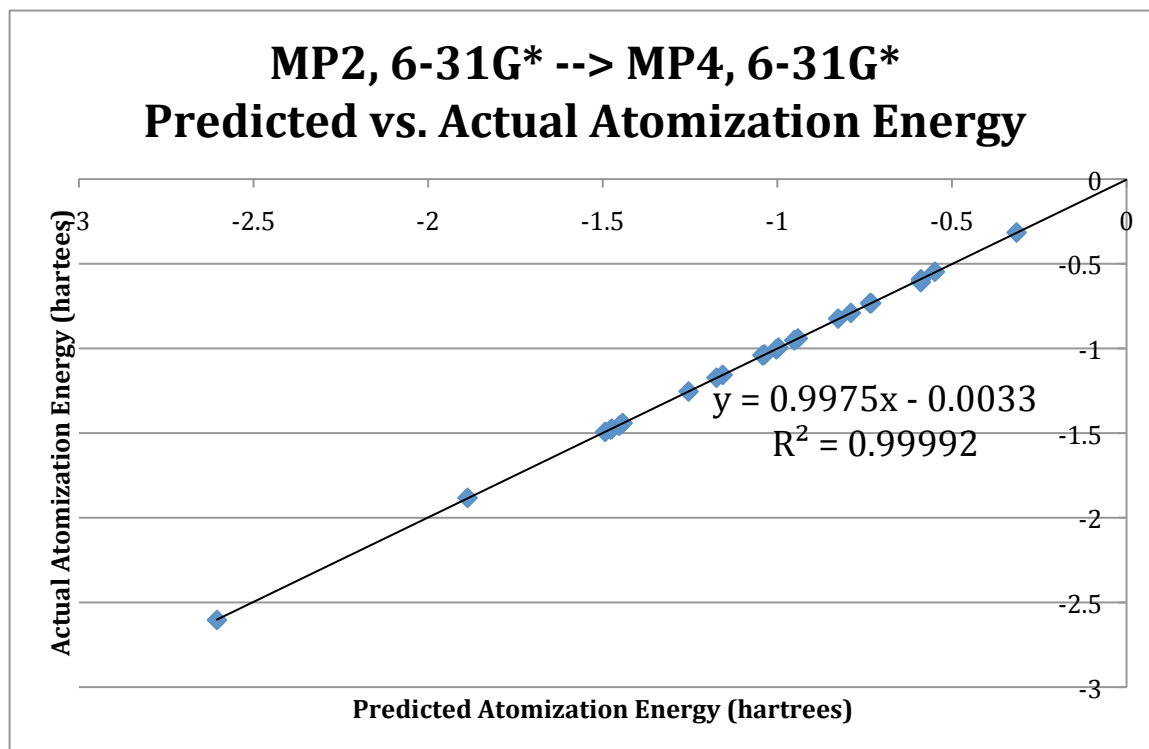


Figure 4: Predicted vs. actual atomization energies for Test 4, in which we corrected from MP2/6-31G\* to MP4/6-31G\*.

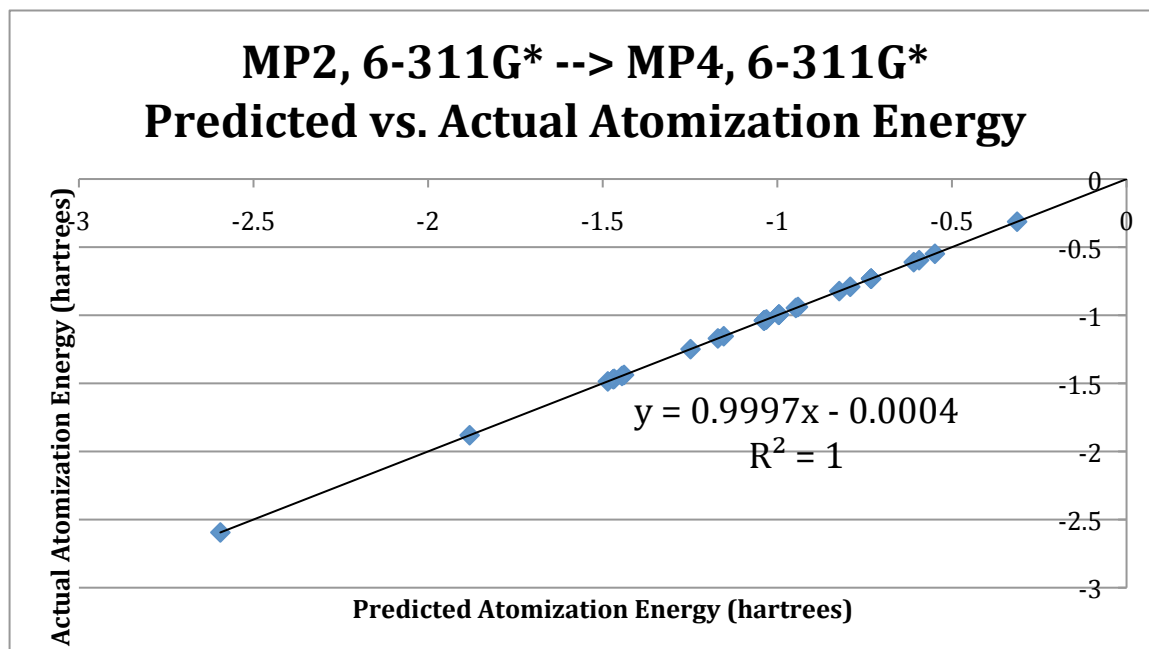


Figure 5: Predicted vs. actual atomization energies for Test 5, in which we corrected from MP2/6-311G\* to MP4/6-311G\*.

CHAPTER 5  
RESULTS PART 3: CORRECTIONS TO MP4/6-311+G(2D,P)

In the final experiment, we chose to correct to MP4, 6-311+G(2d,p) calculations. We chose the same inaccurate methods from experiment 2 – MP2 calculations with the STO-3G, 6-31G\*, and 6-311G\* basis sets (see Table 7). The MP4/6-311+G(2d,p) method is one of the most accurate energy calculations available today, and we hoped to be able to successfully correct to this method from various inaccurate calculations.

Table 7: Summary of Tests 6, 7, and 8 performed in Experiment 3.


Test #	Inexpensive Calculation		Expensive Calculation	
	Computational Method	Basis Set	Improve to: 	Basis Set
6	MP2	STO-3G	MP4	6-311+G(2d,p)
7	MP2	6-31G*	MP4	6-311+G(2d,p)
8	MP2	6-311G*	MP4	6-311+G(2d,p)

Table 8 shows the uncorrected and corrected rms errors in atomization energy and Table 9 lists the bond-based correction factors that were developed in this experiment.

Table 8: Rms error<sup>3</sup> in atomization energy for Tests 6, 7, and 8.

Correction Type	Rms error in Atomization Energy (hartrees)	
	<i>Uncorrected</i>	<i>Corrected</i>
MP2, STO-3G → MP4, 6-311+G(2d,p)	0.09039535	0.00639208
MP2, 6-31G* → MP4, 6-311+G(2d,p)	0.03362057	0.00122973
MP2, 6-311G* → MP4, 6-311+G(2d,p)	0.03654763	0.00155680

Table 9: Bond-based correction factors developed in Tests 6, 7, and 8.

Bond Type	Correction Factors (hartrees)		
	<i>MP2, STO-3G</i> → <i>MP4, 6-311+G(2d,p)</i>	<i>MP2, 6-31G*</i> → <i>MP4, 6-311+G(2d,p)</i>	<i>MP2, 6-311G*</i> → <i>MP4, 6-311+G(2d,p)</i>
C-C	-0.000664989	0.006914062	0.006491094
C-H	0.018166027	-0.009796627	-0.010070717
C=C	-0.011623018	0.006610904	0.006709537
C-O	-0.03694228	0.006094984	0.004460958
C=O	-0.075749648	0.008003379	0.008817802
O-H	-0.041199589	-0.01441106	-0.016332874
C≡C	0.008620853	0.009104089	0.0109364

As evident from Table 8, the correction factors improved the rms error by one order of magnitude in both tests. Furthermore, as evident in the predicted vs. actual atomization energy graphs from Figures 6, 7 and 8, the slopes of the linear fits were 1.0053, 0.9996, and 0.9994 for Tests 6, 7, and 8, respectively. Once again,  $R^2$  values of 0.9997, 0.9999, and 0.9999 display the good fit of each regression line.

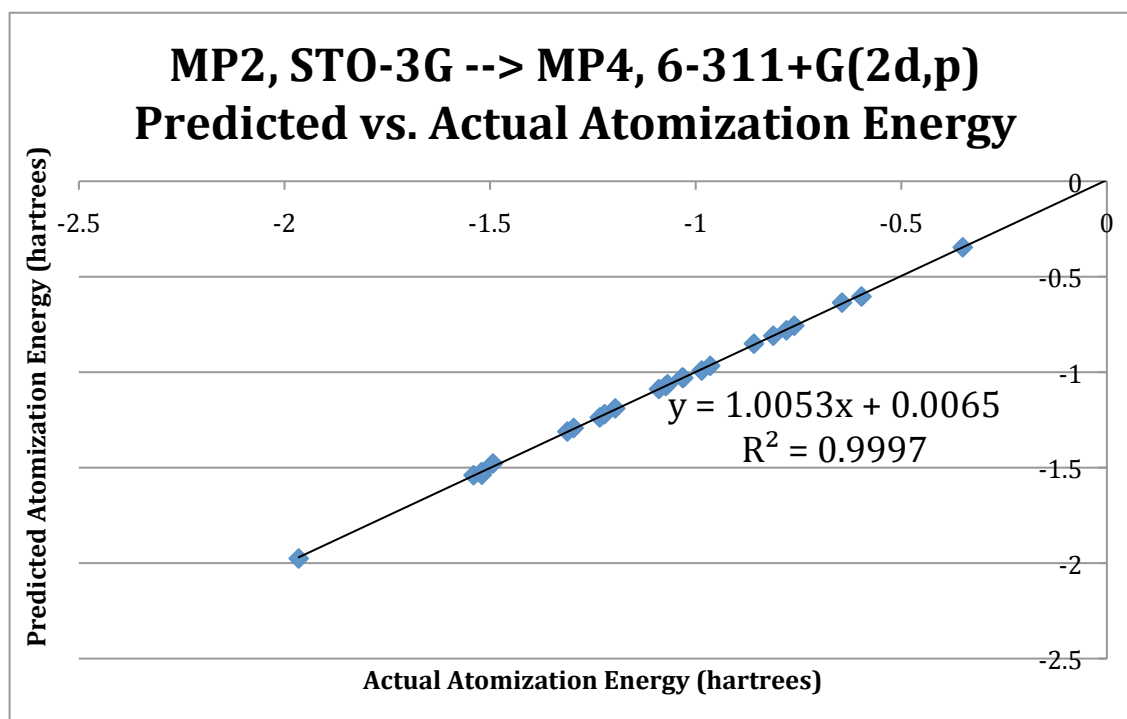


Figure 6: Predicted vs. actual atomization energies for Test 6, in which we corrected from MP2/STO-3G to MP4/6-311+G(2d,p).



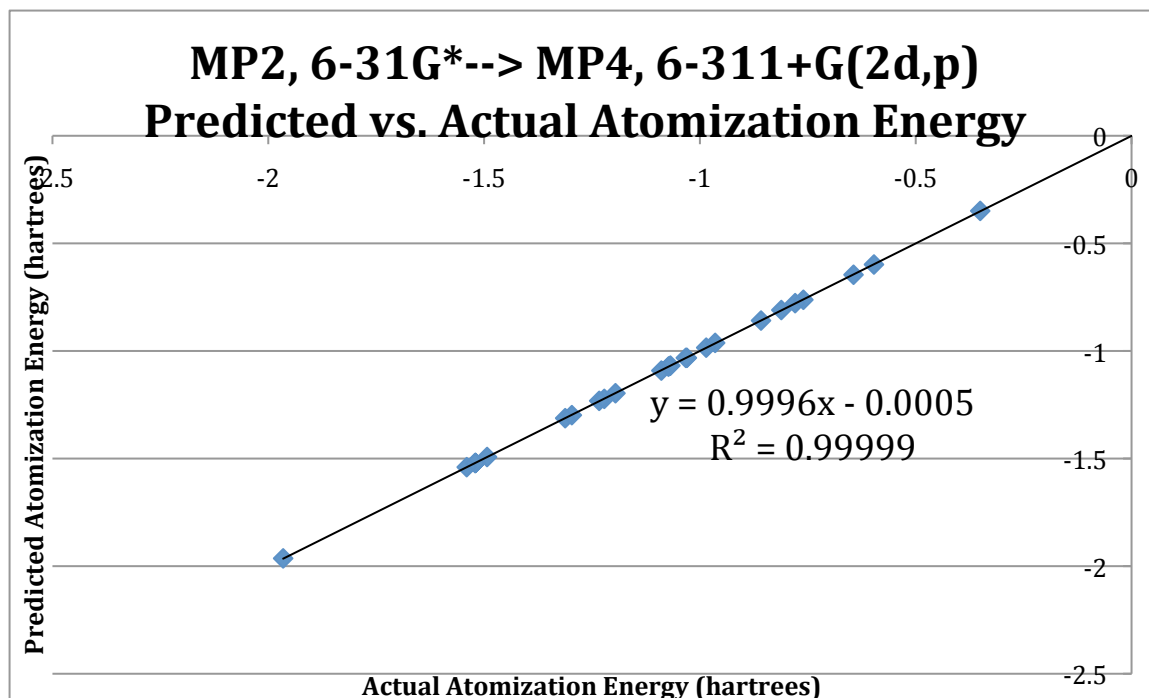


Figure 7: Predicted vs. actual atomization energies for Test 7, in which we corrected from MP2/6-31G\* to MP4/6-311+G(2d,p).

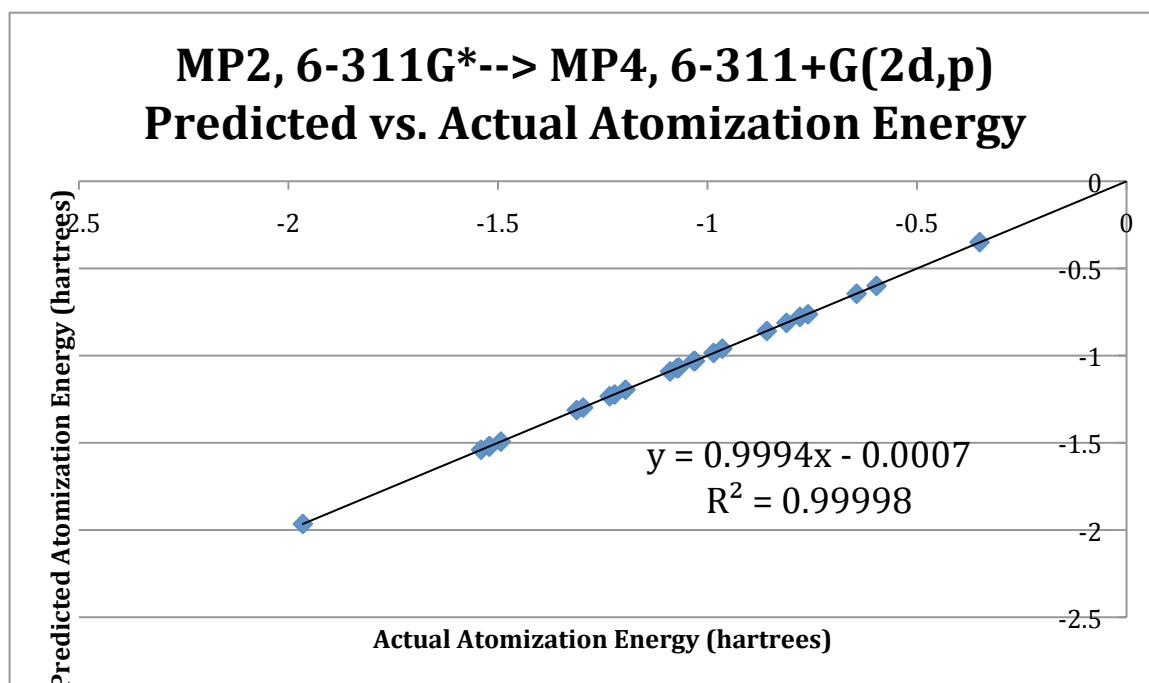


Figure 8: Predicted vs. actual atomization energies for Test 8, in which we corrected from MP2/6-311G\* to MP4/6-311+G(2d,p).

## CHAPTER 6 DISCUSSION

In this project, we used the sum square of errors as an indication of how well the correction factors worked. As evident from Tables 2, 5, and 8, the calculated bond-based correction factors extremely well for all eight tests. They reduced the rms error by as much as two orders of magnitude. The best improvement was in Test 5, in which we corrected from an MP2 to MP4 calculation method using the 6-311G\* basis set. The rms error was reduced from 0.0300197 to 0.00066826 hartrees.

From the predicted vs. actual atomization energy lines, we hoped to find a slope of 1 which would represent perfect corrections. The best line was found in Test 2 with a slope of 1.0000 and an  $R^2$  value of 1.0000. The furthest deviation from this slope was found in Test 6 in which we corrected from an MP2/STO-3G to the MP4/6-311+G(2d,p) calculation with a slope of 1.0053. This is likely due to the fact that this test represented the single biggest improvement in calculation type, not only in calculation method but also in the basis set. STO-3G was the smallest basis set used in the project while the 6-311+G(2d,p) was the largest basis set used. Nonetheless, even this most deviated slope shows fantastic improvements in atomization energy calculations.

Overall, we met our objective to calculate bond-based correction factors to improve the accuracy of inaccurate computational methods to match more accurate methods. For this project, we limited our calculations to molecules with C, H, and O atoms and worked only with atomization energies. Our results showed considerable success. We performed a total of eight tests split into three experiments. In the first experiment, we used a large molecule set and made relatively small improvements in our calculation methods, either improving an MP2 to MP3 or improving just the basis set on the MP2 method. In the second test, we made larger

improvements: MP2 to MP4 using the same basis sets (STO-3G, 6-31G\*, and 6-311G\*) using 25 molecules. Finally, in the third experiment, we used 24 molecules to make corrections to one of the best available calculations: MP4/6-311+G(2d,p). Regardless of the experiment, our calculated bond-based corrections improved the rms error in atomization energy by up to two orders of magnitude.

Such promising results give us reason to believe that similar tests can be conducted with other computational methods and molecules. In the future, we could expand our molecule set to include the nitrogen atom. This would add an extra dimension to our work and allow for our results to be applicable to larger set of molecules.

The field of computational chemistry is already useful in multiple disciplines. Computational calculations are often used in the pharmaceutical industry. Since the process of drug discovery is extremely expensive and time-consuming, computational calculations to model energetics and interactions are often useful in narrowing down potential drug candidates and synthetic routes. Companies like Nimbus Discovery provide computational calculations for pharmaceutical companies to assist them in reducing the amount of time to find a drug candidate.<sup>9,10</sup> However, since even computational methods are time consuming, it would be useful to utilize a quick calculation that could provide results matching an expensive calculation - as we did in our project.

One theoretical question that arises from our project is the applicability of bond-based correction factors in the future. As time progresses, it is inevitable that major breakthroughs will occur in computational chemistry and calculations will become more accurate. We speculate that as computational methods become more accurate, bond-based correction factors will also become more effective in improving calculations. It is likely that further work in this field will

find that tables of correction factors, such as Tables 3, 6, and 9, may be useful for a long time to calculate highly accurate and quick calculations of various molecular properties.

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## LIST OF MOLECULES

<b>EXPERIMENT 1 – TESTS 1, 2</b>	
<ol style="list-style-type: none"> <li>1. methane, CH<sub>4</sub></li> <li>2. ethane, C<sub>2</sub>H<sub>6</sub></li> <li>3. propane C<sub>3</sub>H<sub>8</sub></li> <li>4. n-Butane, C<sub>4</sub>H<sub>10</sub></li> <li>5. isobutane, C<sub>4</sub>H<sub>10</sub></li> <li>6. n-pentane, C<sub>5</sub>H<sub>12</sub></li> <li>7. isopentane, C<sub>5</sub>H<sub>12</sub></li> <li>8. neopentane, C<sub>5</sub>H<sub>12</sub></li> <li>9. hexane, C<sub>6</sub>H<sub>14</sub></li> <li>10. 2-methyl-pentane, C<sub>6</sub>H<sub>14</sub></li> <li>11. 2,2-dimethyl-butane, C<sub>6</sub>H<sub>14</sub></li> <li>12. cyclohexane, C<sub>6</sub>H<sub>12</sub></li> <li>13. cyclopentane, C<sub>5</sub>H<sub>10</sub></li> <li>14. cyclobutane, C<sub>4</sub>H<sub>8</sub></li> <li>15. cyclopropane, C<sub>3</sub>H<sub>6</sub></li> <li>16. ethylene, C<sub>2</sub>H<sub>4</sub></li> <li>17. propene, C<sub>3</sub>H<sub>6</sub></li> <li>18. 1-butene, C<sub>4</sub>H<sub>8</sub></li> <li>19. propyne, CH<sub>3</sub>CCH</li> <li>20. carbon dioxide, CO<sub>2</sub></li> <li>21. formic acid, CH<sub>2</sub>O<sub>2</sub></li> <li>22. acetic acid, C<sub>2</sub>H<sub>4</sub>O<sub>2</sub></li> <li>23. methyl formate, C<sub>2</sub>H<sub>4</sub>O<sub>2</sub></li> <li>24. ketene, C<sub>2</sub>H<sub>2</sub>O</li> <li>25. oxirane, C<sub>2</sub>H<sub>4</sub>O</li> <li>26. acetaldehyde, C<sub>2</sub>H<sub>4</sub>O</li> <li>27. methanol, CH<sub>4</sub>O</li> <li>28. ethanol, C<sub>2</sub>H<sub>6</sub>O</li> <li>29. n-butanol, C<sub>4</sub>H<sub>10</sub>O</li> <li>30. n-pentanol, C<sub>5</sub>H<sub>12</sub>O</li> <li>31. 2-pentanol, C<sub>5</sub>H<sub>12</sub>O</li> <li>32. acetone, C<sub>3</sub>H<sub>6</sub>O</li> <li>33. water, H<sub>2</sub>O</li> <li>34. formaldehyde, H<sub>2</sub>CO</li> <li>35. allene, CH<sub>2</sub>CCH<sub>2</sub></li> <li>36. cyclopropene, C<sub>3</sub>H<sub>4</sub></li> </ol>	<ol style="list-style-type: none"> <li>37. 1,3-butadiene, C<sub>4</sub>H<sub>6</sub></li> <li>38. 1-butyne, C<sub>4</sub>H<sub>6</sub></li> <li>39. 2-butyne, C<sub>4</sub>H<sub>6</sub></li> <li>40. 1,2-butadiene, C<sub>4</sub>H<sub>6</sub></li> <li>41. cyclobutene, C<sub>4</sub>H<sub>6</sub></li> <li>42. methylenecyclopropane, C<sub>4</sub>H<sub>6</sub></li> <li>43. 1-methylcyclopropene, C<sub>4</sub>H<sub>6</sub></li> <li>44. bicyclobutane, C<sub>4</sub>H<sub>6</sub></li> <li>45. isobutene, C<sub>4</sub>H<sub>8</sub></li> <li>46. 2-butene (E), C<sub>4</sub>H<sub>8</sub></li> <li>47. 2-butene (Z), C<sub>4</sub>H<sub>8</sub></li> <li>48. cyclopentene, C<sub>5</sub>H<sub>8</sub></li> <li>49. 1,3-pentadiene (E), C<sub>5</sub>H<sub>8</sub></li> <li>50. 1,4-pentadiene, C<sub>5</sub>H<sub>8</sub></li> <li>51. methylenecyclobutane, C<sub>5</sub>H<sub>8</sub></li> <li>52. spiropentane, C<sub>5</sub>H<sub>8</sub></li> <li>53. ethenylcyclopropane, C<sub>5</sub>H<sub>8</sub></li> <li>54. glyoxal, C<sub>2</sub>H<sub>2</sub>O<sub>2</sub></li> <li>55. 3-methyl-1-butanol, C<sub>5</sub>H<sub>12</sub>O</li> <li>56. 2-methoxy-2-methylpropane, C<sub>5</sub>H<sub>12</sub>O</li> <li>57. 3-methyl-2-butanol, C<sub>5</sub>H<sub>12</sub>O</li> <li>58. 1-methoxy-butane, C<sub>5</sub>H<sub>12</sub>O</li> <li>59. ethyl acetate, C<sub>4</sub>H<sub>8</sub>O<sub>2</sub></li> <li>60. 1,4-dioxane, C<sub>4</sub>H<sub>8</sub>O<sub>2</sub></li> <li>61. 2,3-butanedione, C<sub>4</sub>H<sub>6</sub>O<sub>2</sub></li> <li>62. butyrolactone, C<sub>4</sub>H<sub>6</sub>O<sub>2</sub></li> <li>63. dimethyl ether, C<sub>2</sub>H<sub>6</sub>O</li> <li>64. isopropanol, C<sub>3</sub>H<sub>8</sub>O</li> <li>65. furan, C<sub>4</sub>H<sub>4</sub>O</li> <li>66. propiolactone, C<sub>3</sub>H<sub>4</sub>O<sub>2</sub></li> <li>67. methyl ester-2-propenoic acid, C<sub>4</sub>H<sub>6</sub>O<sub>2</sub></li> <li>68. 2-butenal, C<sub>4</sub>H<sub>6</sub>O</li> <li>69. cyclobutanone, C<sub>4</sub>H<sub>6</sub>O</li> <li>70. 2,3-dihydro-furan, C<sub>4</sub>H<sub>6</sub>O</li> <li>71. vinyl ether, C<sub>4</sub>H<sub>6</sub>O</li> </ol>

**EXPERIMENT 2 – TESTS 3, 4, 5**

1. methane, CH <sub>4</sub>	13. acetaldehyde, C <sub>2</sub> H <sub>4</sub> O
2. ethane, C <sub>2</sub> H <sub>6</sub>	14. methanol, CH <sub>4</sub> O
3. n-Butane, C <sub>4</sub> H <sub>10</sub>	15. ethanol, C <sub>2</sub> H <sub>6</sub> O
4. cyclohexane, C <sub>6</sub> H <sub>12</sub>	16. acetone, C <sub>3</sub> H <sub>6</sub> O
5. cyclopropane, C <sub>3</sub> H <sub>6</sub>	17. water, H <sub>2</sub> O
6. ethylene, C <sub>2</sub> H <sub>4</sub>	18. formaldehyde, H <sub>2</sub> CO
7. propyne, CH <sub>3</sub> CCH	19. allene, CH <sub>2</sub> CCH <sub>2</sub>
8. carbon dioxide, CO <sub>2</sub>	20. cyclopropene, C <sub>3</sub> H <sub>4</sub>
9. formic acid, CH <sub>2</sub> O <sub>2</sub>	21. 1,3-butadiene, C <sub>4</sub> H <sub>6</sub>
10. methyl formate, C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	22. 1,2-butadiene, C <sub>4</sub> H <sub>6</sub>
11. ketene, C <sub>2</sub> H <sub>2</sub> O	23. cyclobutene, C <sub>4</sub> H <sub>6</sub>
12. oxirane, C <sub>2</sub> H <sub>4</sub> O	24. bicyclobutane, C <sub>4</sub> H <sub>6</sub>
	25. glyoxal, C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>

**EXPERIMENT 3 – TESTS 6, 7, 8**

1. Methane, CH <sub>4</sub>	13. methanol, CH <sub>4</sub> O
2. Ethane, C <sub>2</sub> H <sub>6</sub>	14. ethanol, C <sub>2</sub> H <sub>6</sub> O
3. n-Butane, C <sub>4</sub> H <sub>10</sub>	15. acetone, C <sub>3</sub> H <sub>6</sub> O
4. cyclopropane, C <sub>3</sub> H <sub>6</sub>	16. water, H <sub>2</sub> O
5. ethylene, C <sub>2</sub> H <sub>4</sub>	17. formaldehyde, H <sub>2</sub> CO
6. propyne, CH <sub>3</sub> CCH	18. allene, CH <sub>2</sub> CCH <sub>2</sub>
7. carbon dioxide, CO <sub>2</sub>	19. cyclopropene, C <sub>3</sub> H <sub>4</sub>
8. formic acid, CH <sub>2</sub> O <sub>2</sub>	20. 1,3-butadiene, C <sub>4</sub> H <sub>6</sub>
9. methyl formate, C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	21. 1,2-butadiene, C <sub>4</sub> H <sub>6</sub>
10. ketene, C <sub>2</sub> H <sub>2</sub> O	22. cyclobutene, C <sub>4</sub> H <sub>6</sub>
11. oxirane, C <sub>2</sub> H <sub>4</sub> O	23. bicyclobutane, C <sub>4</sub> H <sub>6</sub>
12. acetaldehyde, C <sub>2</sub> H <sub>4</sub> O	24. glyoxal, C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>

## ACADEMIC VITA

### NEELABH MAHESHWARI

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#### Education

Pennsylvania State University, University Park  
BS in Chemistry  
Schreyer Honors College  
Braddock Scholar

*Graduation 2012*

#### Skills

- Fluent in English, Hindi, Spanish, and Urdu.
- Fluent in computer programming languages: C++, FORTRAN.

#### Research Experience

1. **Location:** Penn State Hershey Medical Center, Cancer Institute

**Duration:** June 2011 – Present

**Topic:** Retrospective Study of Radiation Therapy for Prophylaxis of Heterotopic Ossification

**Role:** Designed the study, conducted research, communicated with PSU Institutional Review Board to ensure ethical and legal guidelines were met.

**Abstract:** Heterotopic ossification is a debilitating disease affecting patients who have experienced physical traumatic injuries such as fractures of the hip, shoulder, and elbow. Radiation therapy within a few days of trauma surgery is used for prophylaxis of heterotopic ossification. The outcomes, however, are unclear. Despite preventative actions, many patients develop heterotopic ossification within one year of radiation therapy. Therefore, research needs to be conducted to analyze the effectiveness of the current radiation plans. We will attempt to determine patient risk factors (previous injuries, arthritis) that could increase the risk for heterotopic ossification. Furthermore, we will aggressively study how treatment variables (use of NSAIDs, time interval between radiation and surgery, radiation dosage, etc.) impact patient outcomes. We hope to gain an in-depth understanding of how a multitude of factors effect heterotopic ossification development.

2. **Location:** Penn State Hershey Medical Center, Cancer Institute

**Duration:** June 2011 – August 2011

**Topic:** Comparison of Outcomes of Patients with Stage I Non-Small Cell Lung Cancer Treated with Resection or Stereotactic Radiosurgery

**Abstract:** The purpose of this study was to compare radiotherapy and surgery for patients with clinical Stage I non-small cell lung cancer. We combined two databases containing 180 patients treated by surgery and 137 patients treated with stereotactic body radiation. We compared overall survival, disease-free survival, and locoregional control between the two patient sets. Our study demonstrated similar disease free survival rates and locoregional control. However, patients treated with surgery had worse overall survival rates compared to patients treated with radiation.



**Role:** Student researcher in large, multi-institutional study.

**Achievements:** Paper submitted to *Journal of Clinical Oncology*:

**Title:** Matched-Pair Comparison of Outcome of Patients with Clinical Stage I Non-Small Cell Lung Cancer Treated with Resection or Stereotactic Radiosurgery

**Authors:** J. Varlotto, A. Fakiris, J. Flickinger, L. Medford-Davis, A. Liss, J. Shelkey, C. Belani, J. DeLuca, A. Recht, **N. Maheshwari**, M. DeCamp

3. **Location:** Penn State University, Department of Chemistry

**Duration:** September 2010 – Present

**Topic:** Bond Based Corrections to Improve Atomization Energy Calculations

**Role:** Designed the study, conducting research

**Abstract:** Presently there exist many computational methods that use quantum mechanics to calculate electronic structure and energies of molecules. However, for most systems, such calculations are only approximations and there is a large cost (in time) if we attempt to improve these approximations for more accurate results. We hypothesize that we can improve the accuracy of “cheap” calculations by formulating a list of bond-based correction factors. Our theoretical methods include minimizing multi-dimensional curves by using Monte-Carlo methods. Our goal is to attain highly accurate calculations by adding correction factors to cheap, inaccurate calculations.

**Achievements:** Schreyer Honors College Thesis

**Drug Awareness Program in India**

July 2007 – Present

- Founded a drug abuse/awareness program in a rural village in India (Bahjoi, India) in 2007
- Identified problems - opium and marijuana abuse amongst impoverished families.
  - Opium is grown in many parts of Northern India and although controlled, it often leaks out into surrounding communities hurting families that are already impoverished.
- Designed a 3-week program to address this issue and delivered informational and leadership lectures to middle school students in a school called “Anglo Vedic Convent School” or AVCS.
- Expanded this program to different schools in surrounding area over the past 5 years.
- Founded a chapter of North South Foundation at AVCS, an international organization that provides full scholarships to bright students who cannot afford post-secondary education.
- Awarded 3 scholarships in 2011. Awarded 19 scholarships in 2012.

**Penn State UHS (University Health Center) Intern**

August 2009 – Present

- **Emergency Medical Technician (EMT BCertified)**
  - Provided emergency medical services via ambulatory and on-site care.
- **Leadership Position: “HealthWorks” Team Leader**
  - My team’s objective was to promote awareness and knowledge of health issues such as sexual health, nutrition and fitness, and drugs and alcohol to college students.
  - Advocated healthy lifestyle choices by providing health education programs, information, and materials to students. For example, we organized a weeklong fair called “Green Health Week” for students and faculty.
  - Personally delivered hour-long lectures to college students on these health issues.