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Prediction of keto/enol tautomerism using computational methods

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Prediction of keto/enol tautomerism using computational methods

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Dedication

This thesis is dedicated to my parents, without whose support and aid, in easy and rough, this accomplishment would never have been possible.

This thesis is dedicated to my brother and sister, siblings and friends, may their lives be prosperous and may their achievements echo.

This thesis is dedicated to my grandmother, a second mother, and to the soul of my grandfather, both from whom my requests were never faced with a no.

This thesis is dedicated to what has been, what is being, what could have been, and what is to come.

Declaration

I certify that this thesis is submitted for the degree of master, is the result of my own research, except where otherwise acknowledged, and that this study has not been submitted for a higher degree to any other university or institution.

Signed: ____________________

Anas Omar Yusuf Najjar

Date: 22/12/2019

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Abstract

The measurement of keto/enol tautomerism ratios is a challenging endeavour which has had many different methods throughout history starting from bromine titration and leading to computational methods today. However, there is a vastly large amount of computational methods to choose from, and no real idea as to which method is the best for finding the keto/enol tautomerism ratios. This study applied the use of seven of the most commonly used functionals by researchers on 52 compounds to find the optimal functional, basis set, and solvation cavity for keto/enol tautomerism. However, many of the results obtained from the literature are for neat solutions and, hence, cannot be solvated and were compared to gas phase results. The results obtained showed that the best of the most commonly applied functionals is B3LYP used in tandem with 6-31G basis set and for solvation the Bondi cavity proved to be the most accurate. There is still further research to be conducted as to compare this functional and its basis set combination with other newer functionals that are not very common.

قياس نسبة الكيتون إلى الإينول باستخدام الأساليب المحوسبة

إشراف الأستاذ الدكتور رفيق قرمان

إعداد الطالب: أنس عمر يوسف النجار

الملخص

تعتبر عملية قياس نسبة الكيتون إلى الإينول لخليط متجانس لنفس المادة عملية صعبة الأمر الذي دعا بدوره إلى تطوير العديد من المنهجيات والتجارب على مر التاريخ بداية بالمعايرة الكيميائية بمساعدة البروم وانتهاءاً بالأساليب المحوسبة بمساعدة برامج الكيمياء الكمية. لكن، وبالرغم من توفر عدد كبير من الخيارات المتاحة لقياس النسب بمساعدة الحاسوب، إلا أن تحديد الأسلوب الأمثل يشكل معضلة أمام الباحث.

تبحث هذه الدراسة إمكانية تطبيق الأساليب السبعة الأكثر إنتشاراً في حسابات الكيمياء الكمية في تحديد نسبة الكيتون إلى الإينول وذلك إستعانةً ب52 مركباً سبق وتم تحديد ونشر نسب مكوناتها مخبرياً ومقارنتها بنتائج الحساب الكمي لهذه الدراسة. كما وتبحث إمكانية تحديد "فجوة المحلول النظرية" الأمثل. لكن من الجدير ذكر أن العديد من المركبات التي تم نشر نسبها سابقاً كانت نقية وليست ضمن نظام محلول، مما دعا الباحث إلى الاكتفاء بمقارنة الحسابات الكمية للحالة الغازية للمركب مع النسب المنشورة.

توصل البحث إلى كون أسلوب الحساب الكمي (بي 3 لِب –B3LYP) هو الأمثل في تحديد نسبة الكيتون إلى الإينول وخاصة عند توظيف هذا الأسلوب في إطار مجموعة (31-6 جي – 6-31G). كما وتوصل البحث إلى كون (بوندي – Bondi) فجوة المحلول النظرية الأمثل.

تكمن بالرغم من هذه النتائج حاجة إلى مقارنة المزيد من الأساليب الكمية مع النتائج العملية والنظرية للتوصل إلى المنهجية المثلى في تحديد نسب الكيتون والإينول بصورة قابلة للتطبيق على نطاق أوسع.

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List of Abbreviations

Abbreviation	Meaning
NMR	Nuclear magnetic resonance
H	Enthalpy
S	Entropy
T	Temperature
G	Gibbs free energy
K_T	Tautomerism equilibrium constant
SCF	Self-consistent field
LCAO	Linear combination of atomic orbitals approximation
DFT	Density functional theory

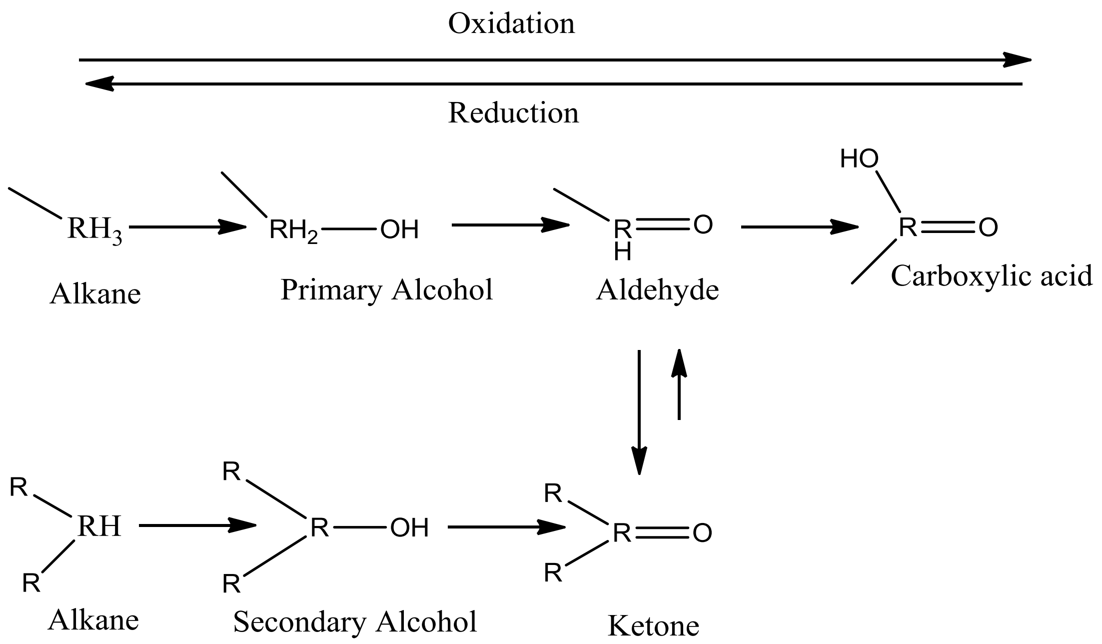
Chapter One

Introduction

1. Introduction

Saving time and cost has been the aim of software ever since their inception; especially in chemistry. If one is to apply theoretical models and software to a given reaction, one would, arguably, save time and, definitely, save resources. However, this endeavour is not as easy as it looks since in chemistry theoretical models have grown exponentially giving researchers a wide variety of models and combinations from which to choose from. This study deals with employing theoretical models and software to calculate the keto-enol tautomerism of ketones and enols.

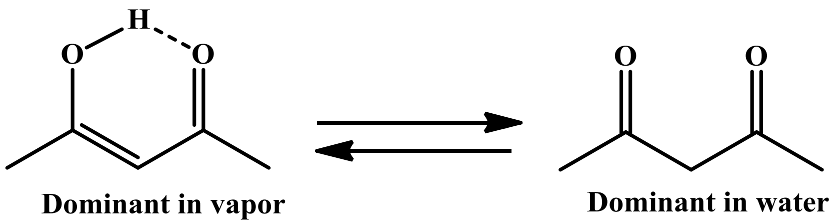
Firstly, in order to describe enols and ketones, one should start from alkanes, the simplest form of organic compounds. The oxidation of the primary carbon would yield a primary alcohol, further oxidation would yield an aldehyde, and further oxidation would yield a carboxylic acid. Similarly, oxidation of a secondary carbon in an alkane would yield a secondary alcohol, and further oxidation would yield a ketone. This is shown in Scheme 1.1. Ketone/enol tautomerism, better known simply as keto-enol tautomerism or tautomerization, is a spontaneous equilibrium explained in section 1.1.



Scheme 1.1: Oxidation/ Reduction of Alkanes, showing Ketone/Enol Tautomerism

1.1 Keto-Enol Tautomerism

Tautomerism, or protropic tautomerism, has been defined as "the addition of a proton at one molecular site and its removal from another"[1]. This definition clearly distinguishes tautomerism or tautomerization from ionization and is an important phenomenon, even though that it occurs in a small number of molecules. Tautomerization is often rapid, dynamic, and sensitive to conditions such as pH, temperature, and solvents. This often makes it hard to isolate one tautomer from another, as well as, idealizing the conditions under which to attempt this isolation. In Scheme 1.2 for example, acetylacetone, the simplest β-diketone available, is influenced by solvent as in that the diketo form is dominant in water whereas in vapour the enol form is dominant.



Scheme 1.2: Acetylacetone and its change in dominance in accordance to solvent.

To first understand the work carried out in this study one must, firstly, look at the theory employed in the software used without delving into too much detail, and later understand how the software is fed the theory. Firstly, the calculation of keto-enol tautomerism is described, followed by an introduction of the theoretical models; their inception and mathematical form. Then, a description the models used in this study.

1.2 Calculation of keto-enol tautomerism

In order to calculate the keto-enol ratio, one must know the concentration of each at a variety of conditions such as temperatures, pHs, solvents, etc… The general formula is that of any given reaction, given that one reactant gives one product, here shown in equation 1.1. The equation is given when one measures the concentration of the enol, but usually as mentioned before the dominant form is the ketone, hence, one would measure the ketone concentration. The equation would, similarly, be given in terms of the ketone concentration.

$$K_T = \frac{[enol]}{[ketone]} = \frac{[enol]}{1 - [enol]}$$

Equation 1.1: The Keto-enol tautomerism equilibrium constant (K_T) as given in terms of enol and ketone concentrations.

In older methods, such as titration, and newer methods, such as nuclear magnetic resonance (NMR) where chemical shifts are measured, both mentioned in the literature review section, the result would be the concentration of the enol (or ketone) and would be given as a percentage. The calculation of which would be simply given as:

$$Enol\% + Ketone\% = 100\%$$

$$Enol\% = 100\% - Ketone\%$$

Equation 1.2: The keto-enol content depicted as percentages.

The calculation using theoretical methods is more complex; since the results of the calculation are thermodynamic parameters. The thermodynamic properties in the calculation output are enthalpy and entropy usually, and combining the parameters with the set temperature of the calculation, the result would be as follows:

$$G = H - TS$$

Equation 1.3: Gibbs free energy in terms of enthalpy (H) entropy (S) and temperature (T)

$$\Delta G = \Delta H - T\Delta S$$

Equation 1.4: The difference in Gibbs free energy in terms of enthalpy, entropy, and temperature defined above.

Both equations give the difference in Gibbs free energy for the reaction. However, in order for this to be related to keto-enol tautomerism, the Arrhenius' equation is applied:

$$K_T = e^{\frac{-\Delta G}{RT}}$$

Equation 1.5: Arrhenius' equation where K_T is the tautomerism equilibrium constant, ΔG is the difference in Gibbs free energy as defined in equation 1.4, R is the gas constant 1.987, and T is the constant temperature of the reaction in Kelvin.

Taking into account equation 1.1, equation 1.5 would provide the concentrations of both reactions in light of the temperature set for the calculation and the output of the calculations.

This, in turn, leads us to the theoretical models.

1.3 Theoretical models

All theoretical models stem from the Schrödinger equation (Equation 1.6) which describes molecules as collections of nuclei and electrons without reference to chemical bonds. The solution to this equation is in terms of the motion of electrons, which in turn, shape the molecular structure and energy as well as bonding. However, one should also mention that while most theoretical models applied today stem from the Schrödinger equation and apply quantum mechanics in the calculations, there are molecular mechanics models which are faster and provide crude results and structures for quantum mechanical calculations. These molecular mechanics calculations do not apply the Schrödinger equation but simply Newton's second law of motion. This entails the depiction of atoms as 'balls' and chemical bonds as 'springs' without properly taking into account complex nuclear details such as atomic and electron orbitals.

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

Equation 1.6: The Schrödinger equation

Where i is the imaginary unit, $\hbar \frac{d}{dt}$ is the reduced Planck constant, Ψ is the state vector of the quantum system, and $\hat{H}$ is the Hamiltonian operator. The Schrödinger equation, as is mentioned above, describes molecules in terms of interaction between electrons and nuclei. Molecular geometry is merely the minimal energy arrangement of those nuclei [2].

Simplifications of the Schrödinger equation are of course necessary for it to be applicable, hence, it can be simply expressed as Equation 1.7:

$$\hat{H}\Psi = E\Psi$$

Equation 1.7: A simplification of the Schrödinger equation

Here, in this simplification, Ψ is a many-electron wavefunction and $\hat{H}$ is the Hamiltonian operator, which when given in atomic units is expressed in Equation 1.8:

$$\hat{H} = -\frac{1}{2}\sum_{i}^{electrons}\nabla_i^2 - \frac{1}{2}\sum_{A}^{nuclei}\frac{1}{M_A}\nabla_A^2 - \sum_{i}^{electrons}\sum_{A}^{nuclei}\frac{Z_A}{r_{iA}} + \sum\sum_{i<j}^{electrons}\frac{1}{r_{ij}} + \sum\sum_{A<B}^{nuclei}\frac{Z_A Z_B}{R_{AB}}$$

Equation 1.8: The Hamiltonian operator expressed in atomic units

Where Z is the nuclear charge, M_A is the ratio of mass of nucleus A to the mass of an electron, R_{AB} is the distance between the nuclei A and B, r_{ij} is the distance between electrons i and j, and r_{iA} is the distance between electron i and nucleus A.

However, and even after some simplification, the Schrödinger equation can only be solved for a single electron system, i.e. the hydrogen atom, and cannot be solved to this day even for a simple two electron system such as the helium atom. Hence, approximations had to be made to make use of the equation. Thus, all quantum chemical models available to us today are but mere approximations, and good ones at that, which can interpret theoretically the molecular structure, isolate intermediate states, and interpret intramolecular forces to say the least. Quantum chemical models differ in the nature of these approximations, and differ in their capability, reliability, and time and computer power needs.

1.3.1 The Born-Oppenheimer approximation

This could be thought of as the first approximation to the Schrödinger equation. In this approximation which Max Born and J. Robert Oppenheimer proposed in 1927 [3] they proposed that since the movement of the nucleus is much slower than that of the electron it could be taken out of the equation and, thus, considered the movement of the nuclei as zero. This resulted in Equation 1.9 below:

$$\hat{H}^{el} = -\frac{1}{2}\sum_{i}^{electrons}\nabla_i^2 - \sum_{i}^{electrons}\sum_{A}^{nuclei}\frac{Z_A}{r_{iA}} + \sum\sum_{i<j}^{electrons}\frac{1}{r_{ij}}$$

Equation 1.9: The Born-Oppenheimer approximation expressed in atomic units

Here we notice from their approximation the deletion of the term in Equation 1.9 above describing the nuclear kinetic energy as it is zero. While the movement of nuclei is in fact "slow" and not zero, the Born-Oppenheimer approximation appears to be valid in the calculation of molecular structure and relative energies, nonetheless.

1.3.2 The Hartree-Fock Approximation

In 1928, a mere year after the publication of the Schrödinger equation, Douglas Hartree formulated what is known as the Hartree equations [4-6]. In essence, and since the Schrödinger equation can be calculated for a single particle, Hartree proposed that calculating the solutions to the Schrödinger equation for each electron independently and then sum them up we should expect to come up with at least an approximation. Also, Hartree proposed that each nucleus with its electrons formed a spherically symmetric field or what we know as "self-consistent field" (SCF). Nearly, if not all, calculations used today apply the SCF procedure in their molecular calculations. The SCF procedure can be summarized in Equations 1.10 and 1.11 in the form of:

$$f(i)\,\chi(\mathbf{x}_i) = \varepsilon\chi(\mathbf{x}_i)$$

$$f(i) = -\frac{1}{2}\nabla_i^2 + \upsilon^{eff}(i)$$

Equations 1.10 and 1.11: The Hartree-fock equations.

Where the first is the actual equation and the second is the Fock operator. Here x_i are the spin and spatial coordinates of electron i, χ are the spin orbitals, and υ^{eff} is the effective potential as seen by electron i.

1.3.3 Linear combination of atomic orbitals approximation (LCAO)

The Hartree-Fock approximation consist of two coupled differential equations each involving the coordinates of a single electron. The LCAO approximation introduces an addition approximation in order to transform the Hartree-Fock equations into a set of algebraic equations.

The first introduction of this approximation was by Sir Kohn Lennard-Jones in 1929 [7] and assumes the existence of quantum superposition of atomic orbitals called molecular orbitals. The main assumption was that since in Hartree-Fock approximations many electron solutions will be an approximation of a single electron solution (i.e. the hydrogen atom), then perhaps molecular solutions are made up of atomic solutions.

The equation proposed assumed that the number of molecular orbitals is equal to the number of atomic orbitals. Hence, the expression for the molecular orbital would be:

$$\phi_i = \sum_r c_{ri}\chi_r$$

Or

$$\phi_i = c_{1i}\chi_1 + c_{2i}\chi_2 + c_{3i}\chi_3 + \cdots + c_{ni}\chi_n$$

Where Ø is the so-called basis functions and χ are the spin orbitals.

Equation 1.12: The LCAO approximation expression

1.3.4 Roothaan-Hall equations

Developed independently by Clemens C. J. Roothaan [8] and George G. Hall [9] in 1951, the Roothaan-Hall equations are basically a combination of both the Hartree-Fock approximations and the LCAO approximations in light of the Schrödinger equation. The main equation is shown below:

FC=εSc where ε is the orbital energies, S is the overlap matrix, and F is the Fock-matrix and C is a matrix of coefficients.

$$F_{\mu\nu} = H_{\mu\nu}^{core} + J_{\mu\nu} - K_{\mu\nu}$$

Where H is the Hamiltonian explained below

$$H_{\mu\nu}^{core} = \int \phi_\mu(\mathbf{r}) \left[-\frac{1}{2}\nabla^2 - \sum_{A}^{nuclei} \frac{Z_A}{r} \right] \phi_\nu(\mathbf{r})\, d\mathbf{r}$$

$$J_{\mu\nu} = \sum_{\lambda}^{basis\ functions} \sum_{\sigma} P_{\lambda\sigma}\,(\mu\nu \mid \lambda\sigma)$$

Where $J_{\mu\nu}$ are the Colomb elements and P is the density matrix shown below

$$K_{\mu\nu} = \frac{1}{2} \sum_{\lambda}^{basis\ functions} \sum_{\sigma} P_{\lambda\sigma}\,(\mu\lambda \mid \nu\sigma)$$

Where $K_{\mu\nu}$ are the exchange elements

$$P_{\lambda\sigma} = 2 \sum_{i}^{\text{occupied molecular orbitals}} c_{\lambda i} c_{\sigma i}$$

and finally

$$(\mu\nu \mid \lambda\sigma) = \iint \phi_\mu(\mathbf{r_1})\phi_\nu(\mathbf{r_1})\left[\frac{1}{r_{12}}\right]\phi_\lambda(\mathbf{r_2})\phi_\sigma(\mathbf{r_2})d\mathbf{r_1}d\mathbf{r_2}$$

The two electron integrals.

Equations 1.13-1.19: The Roothaan-Hall equations

Nowadays, all methods resulting from the solution of the Roothaan-Hall equations are termed Hartree-Fock models. The term *ab initio* was once used to describe those models, however, presently they are used to describe non-empirical attempts to solve the Schrödinger equation. Today, Hartree-Fock models are used to calculate for molecules 50-100 atoms in size.

1.3.5 Kohn-Sham equations and density functional theory methods (DFT)

Density functional theory methods deal more with the energy of electrons and their density as opposed to the wavefunction based approach. They do, however, have their similarities. Firstly, DFT methods and the wave theory methods deal with a single electron matrix and secondly, both the electron density, employed by DFT, and the SCF approach require nearly identical matrix elements.

DFT or Kohn-Sham equations, named after W. Kohn and L. J. Sham [10], were devised in 1965 and are based on the fact that the sum of the exchange and correlation energies of a uniform electron gas can be calculated knowing only its density. For his discovery, Walter Kohn was awarded the Nobel Prize in Chemistry in 1998. They devised a simple equation where:

$E = E_T + E_V + E_J + E_{XC}$

Equation 1.20: the main DFT equation where E is the electron energy total, E_T is the kinetic energy, E_V is the nuclear interaction energy, E_J is the Coulomb energy, and E_{XC} is the exchange/correlation energy.

Except for E_T all components depend on the total electron density shown below:

$$\rho(\mathbf{r}) = 2 \sum_{i}^{\text{orbitals}} \left|\psi_i(\mathbf{r})\right|^2$$

Equation 1.21: Total electron density equation in DFT models

Modern DFT methods divide the calculation into two parts; the first which involves everything but the exchange/correlation part and the second which calculates it using conventional Hartree-Fock models. These classical DFT methods are not used as widely as once they were, examples such as BP [11], BLYP, and EDF1 models [12], have been superseded by hybrid functional such as the popular B3LYP.

One example of how DFT models differ in their definition of the electron energy total is that B3LYP defines exchange energies using slater and Hartree-Fock approximations while it defines correlation energies using LYP and VWN functional III [13]. In turn, M06 for example incorporates spin density, spin gradient, and spin kinetic energies of electrons in its approximation and uses a VSXC functional [14].

1.3.6 Hybrid Functionals

Hybrid functionals, at their essence, employ the DFT theory but for one aspect: E_{XC} is defined differently. The electron exchange/correlation energy is described using both DFT level of theory and HF level of theory. This, in turn, allows for improved description of thermochemistry as well as improved energies of molecular systems [15]. Hybrid functionals used in this study are B3LYP [13], CAM-B3LYP [16], X3LYP [17], M05 [18], M05-2x [19], M06 [14], and M06-2x [14].

1.3.7 Performance and cost

It is not possible to determine how much computing time or power is needed for a certain calculation. We do, however, know that some methods take a lot of time, for example *ab initio* functionals such as the Møller–Plesset perturbation theory sets MP2, MP3 etc…[20] We also know that semi-empirical methods such as PM3 and AM1 take a relatively short times for calculations. Furthermore, hybrid functionals fall within the ‘acceptable’ time vs accuracy range. Table 1.1 [2] shows the task vs the methodology and the result obtained. While the table generalizes the outcome and time cost of each type of calculation, it does not delve into details regarding different functionals available. To my knowledge, and in accordance to my scan of the literature prior to beginning this study, no recommendation has been done on a wide range of molecules for the calculation of keto/enol tautomerization.

Table 1.1: Comparison between different models and applications vs the expected outcome.

task	molecular mechanics	semi-empirical	Hartree-Fock	density functional		LMP2	MP2
				EDF1	B3LYP		
geometry (organic)	F→G	G	G	G	G	N/A	G
geometry (transition metals)	P	G	P	G	G	N/A	F
transition-state geometry	N/A	F→G	G	G	G	N/A	G
conformation	F→G	P	F→G	G	G	N/A	G
thermochemistry (non *isodesmic*)	N/A	P	F→G	G	G	G	G
thermochemistry (*isodesmic*)	N/A	P	G	G	G	G	G
cost	very low	low	moderate	moderate	moderate	high	high

G = good F= fair P = poor N/A = not applicable

1.4 Problem statement

The prediction of keto/enol tautomerism is troublesome due to many factors; Firstly, the tautomerization is affected by conditions such as pH, temperature, solvent, etc… Secondly, history depicted many methods to predict keto/enol tautomerism (this is described in detail in the literature review section). The earlier methods were not accurate enough and were hard to reproduce. Today, the methods available are UV spectroscopy and NMR, both are also affected by the aforementioned factors and are not available, especially NMR, to every researcher due to high cost. Hence, there is need for a quick, time and material saving method which can be reproduced and is not affected by environmental factors. The proposed method is computational calculation of keto/enol tautomerism. However, computational calculation is also hindered by a very broad range of possible options to choose from.

1.5 Study objectives

The primary objective of this study is to test the most commonly used computational methods and basis sets on a large number of molecules with reported experimental keto/enol ratios to find the optimal method and basis set combination capable of predicting keto/enol tautomerism ratios under controlled (computational) conditions with reasonable accuracy.

1.6 Research questions

Before and while performing this study, many questions arose; Firstly, is it possible to find an optimal functional/basis set combination capable of predicting with reasonable accuracy the keto/enol tautomerism ratio computationally without the need for laboratory work? Secondly, which basis set/functional combination provides the best compromise between calculation time and accuracy of keto/enol ratio predicted?

Chapter Two

Literature Review

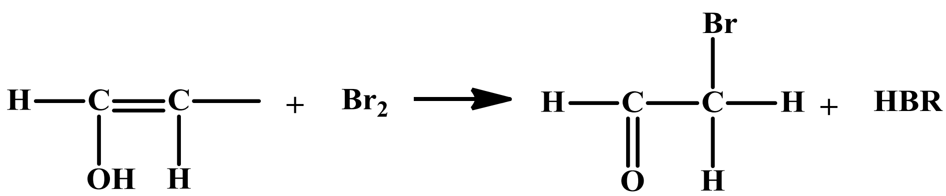
2. Literature review

2.1 History of keto/enol ratio calculation

The methods by which the ratio of enol/ketone was calculated over the years differed through time. It is clear and logical that these methods are limited by the technologies available at the time. Herein is reported the different methods used in order from the oldest to the newest.

2.1.1 Kurt Meyer Method

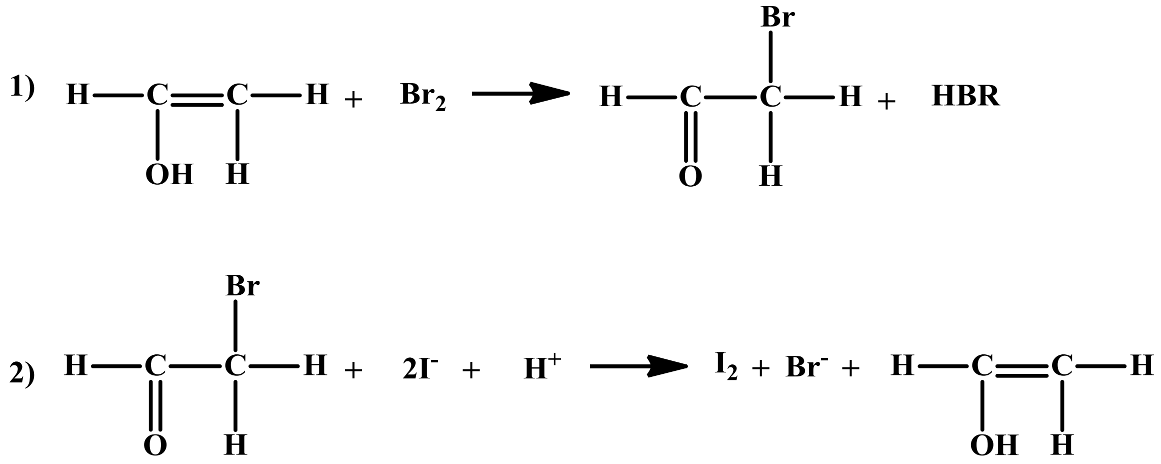
In the earliest papers available, the method of calculating enol ratios was bromination through Kurt Meyer titration. This method was first published in 1911 [21] and it exploited the fact that an enol differs from its keto tautomer in that it has a carbon-carbon double bond, and an ethylenic hydrogen. In Kurt Meyer direct titration (see Scheme 2.1), a bromine solution is added to an aldehyde. This resulted in the reaction between the bromide ion and the carbons on each side of the double bond, forming a carbocation and eventually the binding of bromide to the β-carbon, the formation of a ketone, i.e. the double bond between the α-carbon and the oxygen, and the production of HBr in the process. The end point was determined as the appearance of a yellow colour, which meant that added bromine was not reacting, hence, signalling the end of the reaction.



Scheme 2.1: Kurt Meyer direct bromination

This method, however, had its disadvantages; the bromine titrant was instable and the perception of the end point through the yellow colour was difficult. Hence, Meyer would go on to conjure a more accurate method, and one which he preferred more. In this method, called indirect titration (see Scheme 2.2), the total amount of bromine added to the solution did not matter and an excess was merely added. The results of the reaction were hydrogen bromide, as in the previous method, and monobrominated diketone or ketoester. Later, sodium thiosulfate was quickly titrated to the mixture to remove unreacted bromine followed by the addition of potassium iodide to displace the bromide ion. This resulted in the final product being the original tautomeric mixture of keto and enol forms. Further, thiosulfate was titrated again to produce the milliequivalents of iodine and the milliequivalents of the enol tautomer.

However, this improvement did not quite yet account for excess bromine which would further catalyse the enolization of the keto form. Meyer and Kappelmeier would go on to improve the improved indirect bromination by immediately adding an excess for 2-napthol to remove unreacted bromine. The unreacted 2-napthol would cause no interference with the rest of the steps of the titration [22].



Scheme 2.2: Kurt Meyer indirect bromine titration- first improvement.

However, between the three methods large variations were found. For example, in the calculation of the enol percentage of ethyl acetoacetate while changing the solvent to low temperatures close to 0°C the enol percentage in methanol, benzene, and carbon disulphide were found to be 6.87%, 16.2%, and 32%, respectively [21]. While this modification to the original direct titration method was the preference of Meyer, some criticized his preference and thought that the direct method was more accurate [23].

Later, in 1938, Cooper and Barnes would propose an 'improved Kurt Meyer Titration'[24]. The authors claimed that the indirect titration method suffered from many drawbacks. Firstly, 2-naphthol and its alcoholic solutions are coloured brown, making it difficult to ascertain whether excess bromine had been removed or not. Secondly, the colour causes an error when free iodine is titrated with sodium thiosulfate until the yellow colour is removed. The solution to this problem would be the use of diisobutylene which, according to the authors, would absorb bromine forming a colourless bromide. Also, the diisobutylene would not react with the iodine.

A final modification would follow, Schwarzenbach determined that the enol content is better calculated by running a ketone solution of a known concentration and a bromine solution of steadily increasing concentration at controlled rates through a reaction vessel. Determination of enol would be done by determining the end point potentiometrically [25].

Alexander Gero [26] found that mixed halogens, being polar, were incorporated into the ketone more rapidly than bromine and did not cause substitution. He opted to use iodine monochloride, being the most polar halogen available, rather than bromine in the Kurt-Meyer titration. This, he claimed, proved feasible and a notable improvement on previous titration methods. His method proved to be the most accurate when compared to recent literature, reporting values for several enols. Those are shown in Table 2.1 [27].

Table 2.1: Enol content reported by Alex Gero using mixed halogens method

Ketone	Enol Content %
Ethyl acetoacetate	13.2
Ethyl benzoylacetate	18.5
Acetylacetone	79.7
Camphor	0.123
Acetone	1.5E-4

2.1.2 Precipitation method

While the aforementioned improvements to Kurt Meyer's method proved somewhat satisfactory, especially with the titration proposed by Alex Gero, in 1947 a new method would emerge: precipitation. Seaman et al. would propose that with the careful control of pH an insoluble copper (II) salt may be formed [28]. This is true since most β-dicarbonyl compounds react with copper salts forming chelated insoluble compounds. However, this method proved to be difficult to reproduce since a deviation in less than 1 pH degree would cause different results.

2.1.3 Titration using non-aqueous solvents

In 1948, the development of this method began and was perfected in 1952 by Fritz. This method revolved around the idea that enols can be considered weak acids and, thus, can be titrated as is done to conventional weak acids. This, hence, required the use of a suitable base, an end point, and an indicator. In 1952 Fritz managed to successfully titrate enolic compounds using sodium methoxide as titrant, though, he later recommended the use of potassium methoxide since the end point is sharper than that using sodium methoxide [29, 30]. Compounds such as enols, he states, require the use of azo violet or thymol blue as endpoint indicators depending on the acidity of the enol.

2.1.4 Spectroscopic methods

Since the discovery of spectroscopic methods, they have been used for a variety of applications. The prediction of keto/enol tautomerism ratios is one of them.

2.1.4.1 Infrared (IR)

The earliest reported use of this method to determine the percentage of enols in a tautomeric mixture can be dated back to 1949. In a publication by Le Févre and Welsh an estimation of the enol ratio of ethylene dibromide and pyridine using IR spectroscopy [31] (Figure 2.1). The K values obtained for the compounds were 0.13 and 0.05 respectively where K=[enol]/[ketone]. However, it is apparent from the paper that the optimization of the solvent was critical to the measurements. Moreover, the cell density played part and finding the optimal wave length proved tedious, showing that optimal absorption is achieved at the 1600-1750cm^{-1} range which corresponds with esters and carbonyl compounds making differentiation between the three possible, where the third is apparently the ketone itself.

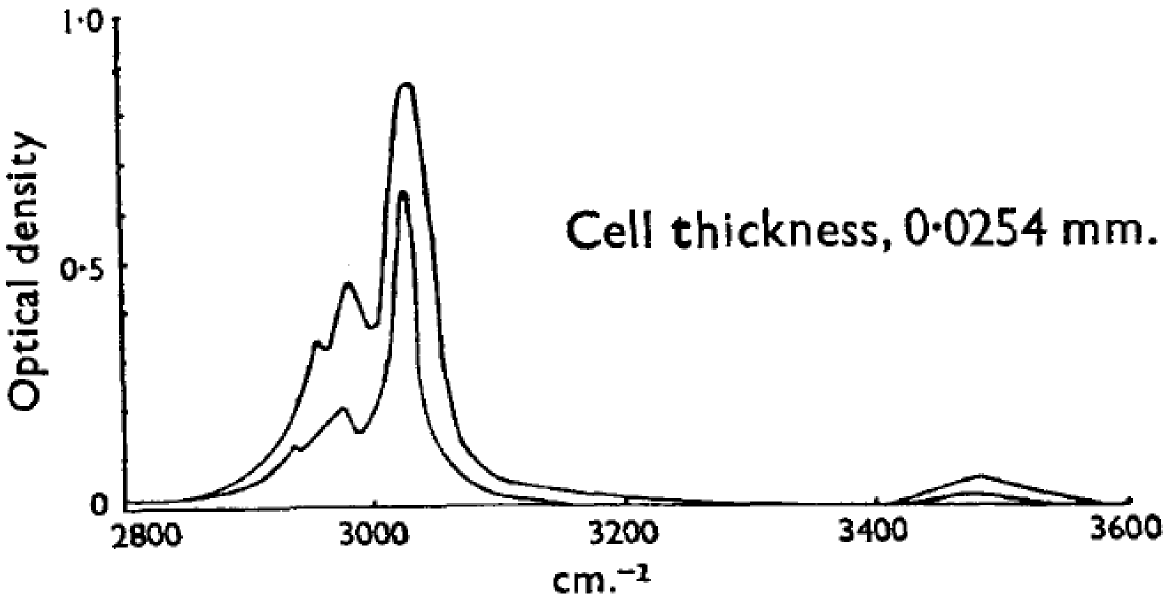


Figure 2.1: IR curves obtained by Le Févre and Welsh where the top curve is pure ester and the lower curve is a 20% solution of ethyl acetoacetate in CS_2

In a later paper by Emsley and Freeman in 1987 [32], confidence in IR readings was revived as the authors had access to both NMR and IR technologies. In a full table, they compare the results obtained by IR and NMR for the enol ratio of pentane-2,4-dione in 21 different solvents. An excerpt from his table is shown below in Table 2.2. His results show clearly that IR is comparable to NMR under the right conditions. It is arguable that his results apply for one single compound, and for a diketone and that smaller, larger, or monoketones cannot deliver such attractive results. This question, to my knowledge and scan of the literature, is unanswered.

Table 2.2: IR vs NMR enol % as reported by Emsley and Freeman for pentane-2,4-dione

Solvent	% enol IR	% enol NMR
C_6H_{12}	97.7	97.0
CCl_4	96.8	94.6
Dioxan	82.6	82.4
Et_2O	96.1	91.9
Ethanol	72.1	74.4

In the 1960s, with the discovery and application of NMR the use of IR to determine enol/ketone ratios died out. Furthermore, due to the fact the IR absorbance is not linearly correlated with concentration, and the many factors that have to be considered before an accurate estimate or measurement of the enol percentage can be achieved, IR will not be making a comeback in this area.

2.1.4.2 Ultraviolet-absorption spectroscopy

Unlike IR spectroscopy, UV spectroscopy has been widely used in the measurement of β-diketones and α-ketones and although the majority of work has been done in solution, we find one important paper that performed this in gas phase which we will later touch on.

In a paper by Zawadiak and Mrzyczek [33] ten compounds were studied. The main aim of the study was to see the effect of substituents, mainly methoxy, on the benzene rings on each side of the β-diketone. The structure of their compound is shown in Figure 2.2. Their main findings, apart from reporting the enol percentage in four different solvents (benzene-d_6, $CDCl_3$, acetone-d_6, and DMSO-d_6), was the effect of the substituent. They report that having a methoxy group in the para position increases absorption in the UV-a range, while having it in the meta position had no effect on the UV spectra. However, having the methoxy group in the ortho position caused steric effects and caused an equilibrium shift towards the ketone. Logically, they conclude, that having two methoxy groups in the para position had the most effect, while have two methoxy groups in the ortho position caused the strongest shift towards the ketone form. This is depicted in Figures 2.3-6

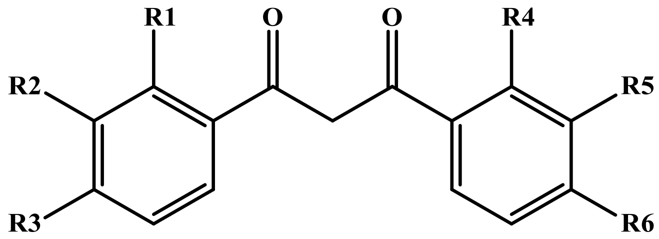


Figure 2.2: Chemical structure of compounds used by Zawadiak and Mrzyczek. R= H or OMe

Table 2.3: Compounds synthesized by Zawadiak and Mrzyczek and their yields.

Formula number	R^1	R^2	R^3	R^4	R^5	R^6	Yield
1	H	H	H	H	H	H	80%
2	OMe	H	H	H	H	H	66%
3	H	OMe	H	H	H	H	69%
4	H	H	OMe	H	H	H	75%
5	OMe	H	H	OMe	H	H	61%
6	H	OMe	H	OMe	H	H	66%
7	OMe	H	H	H	H	OMe	70%
8	H	OMe	H	H	OMe	H	66%
9	H	OMe	H	H	H	OMe	70%
10	H	H	OMe	H	H	OMe	73%

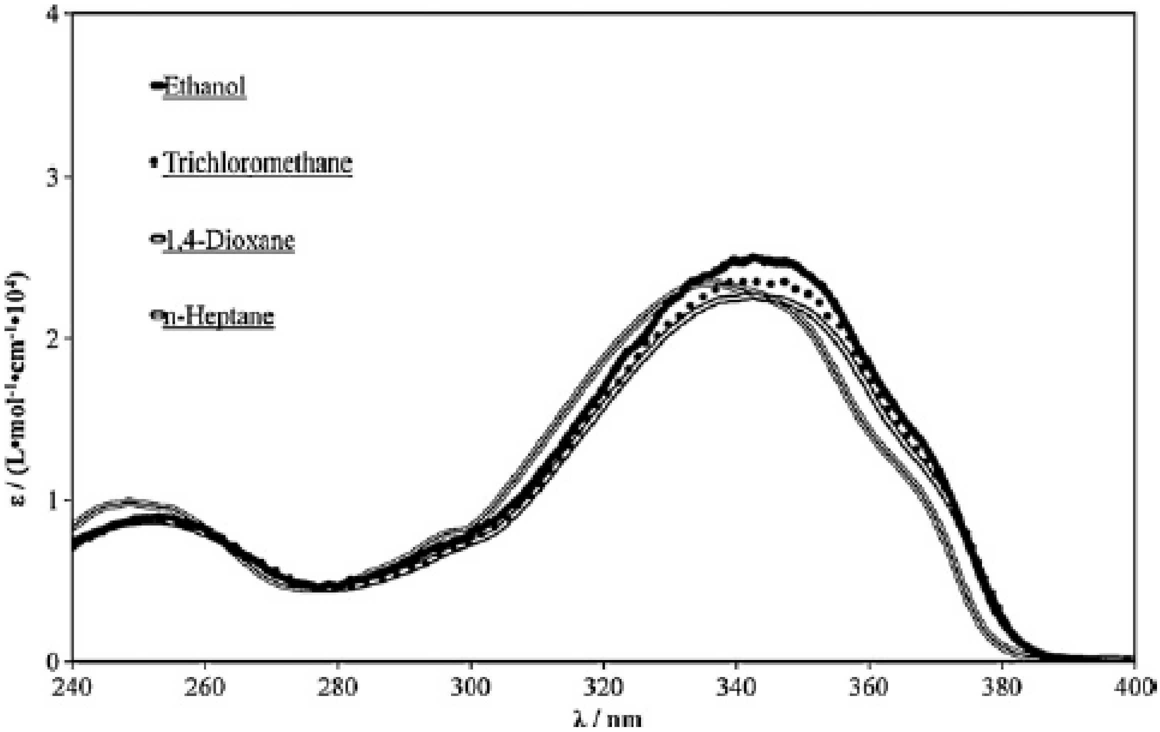


Figure 2.3: UV absorption spectra of compound 1 in ethanol, trichloromethane, 1-4-dioxane, and n-heptane as depicted in the paper by Zawadiak and Mrzyczek.

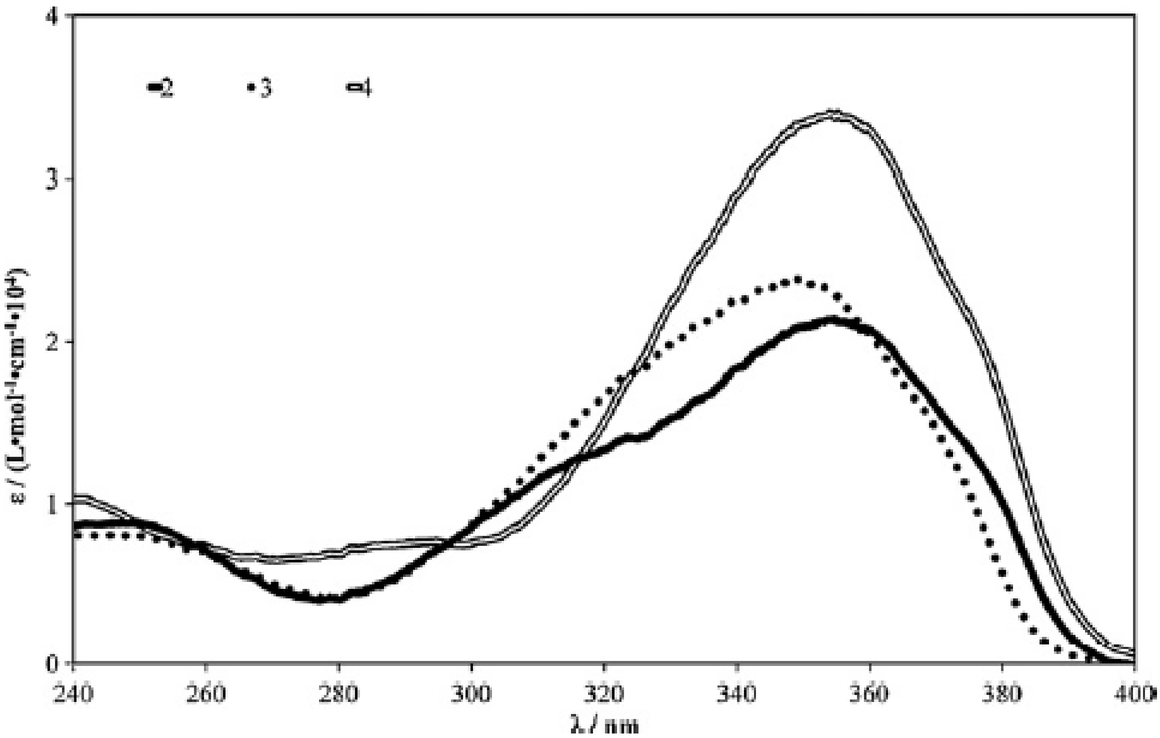


Figure 2.4: UV absorption spectra of compounds 2, 3, and 4, in ethanol as depicted in the paper by Zawadiak and Mrzyczek.

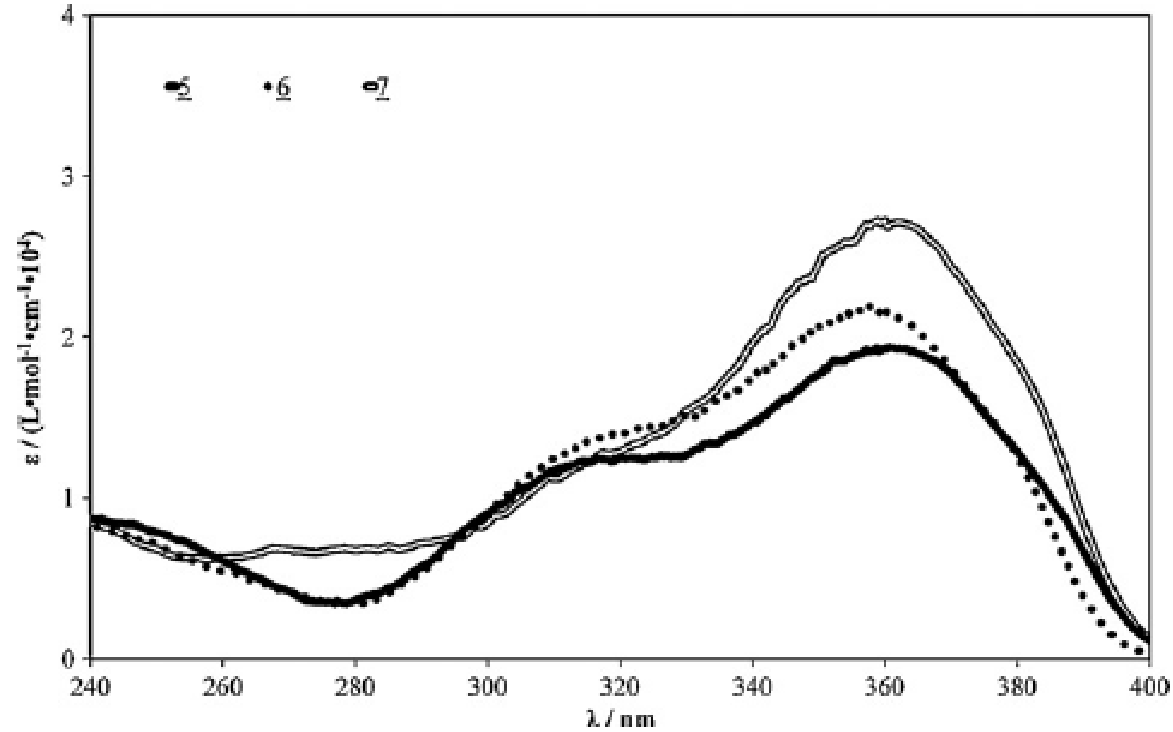


Figure 2.5: UV absorption spectra of compounds 5, 6, and 7, in ethanol as depicted in the paper by Zawadiak and Mrzyczek.

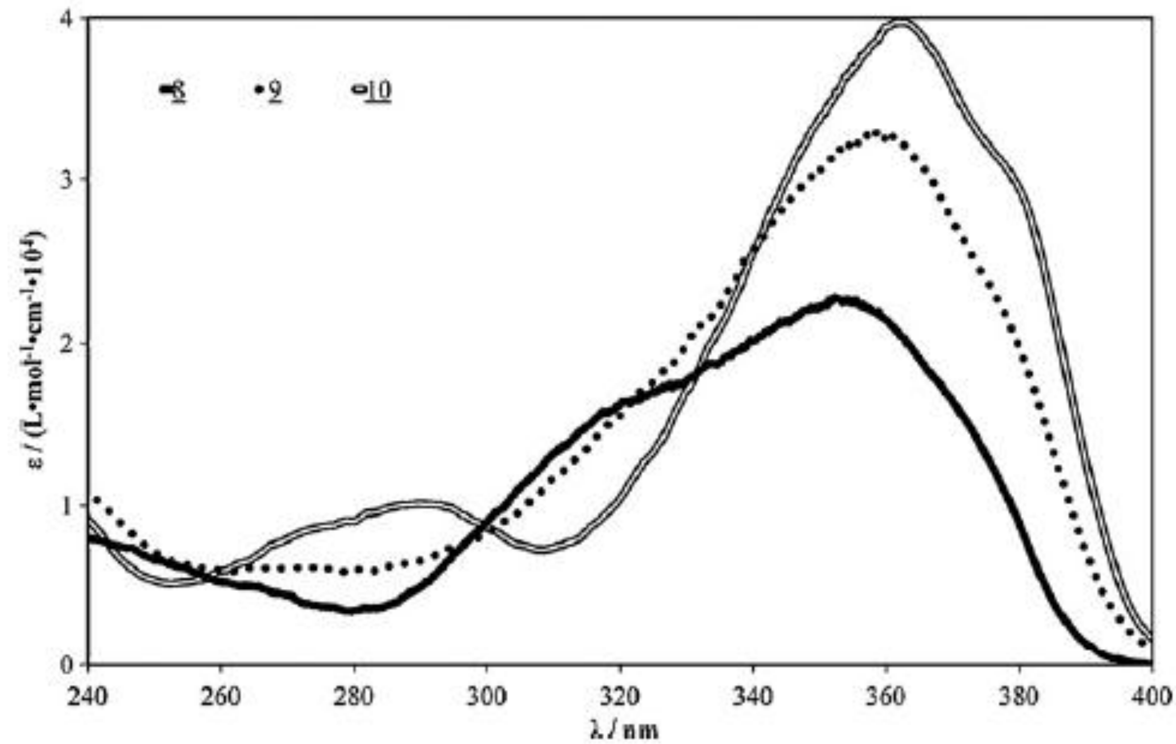
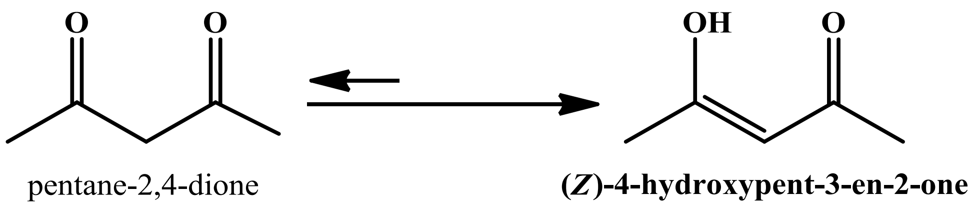


Figure 2.6: UV absorption spectra of compounds 8, 9, and 10, in ethanol as depicted in the paper by Zawadiak and Mrzyczek.

The paper which measured the keto-enol equilibrium in vapor phase was by Hiroshi, Hiroshi, and Saburo [34]. The UV spectra of acetylacetone was obtained at vacuum and measured in the vapor phase and in several organic solvents at various temperatures. The paper also deals with Rydberg excitation bands, CNDO-CI method, and charge-transfer, all of which are irrelevant to the scope of this manuscript.

2.1.4.3 Nuclear magnetic resonance spectroscopy (NMR)

In a paper dated 1953, Jarret, Sadler, and Shoolery obtained proton-NMR resonance signals from a tautomeric mixtures [35]. They succeeded in determining the keto-enol equilibria for 2,4-pentadione (Scheme 2.3) and 3-methyl-2,4-pentadione with high resolution suitable over a range of temperatures. They also compared their results to an earlier paper [36] that used bromine titration, an older method touched upon earlier, with considerable differences. The measurements for 2,4-pentadione enol % were 85% and 76% for NMR and bromination, respectively, and for 3-methyl-2,4-pentadione enol % the measurements were 30% and 31.5% in the same order. Using one of the compounds in their paper, I take the opportunity to explain how the keto/enol ratio is calculated using proton-NMR.



Scheme 2.3: Keto enol equilibrium between pentane-2,4-dione and its enol. The equilibrium favours the enol.

In the above compound there are four structurally non-equivalent kinds of protons in the tautomeric mixture: CH_3, CH_2, CH, and OH. Thus, we expect 4 chemical shifts on the proton-NMR spectrum. The relative area under the curve would be the measurement criteria, for example, since OH and CH are equal in their presence in the mixture, it would be expected that they would produce two chemical shifts of the same area under the curve and can be, thus, eliminated. It would be expected that CH_3 bearing the most abundant form of hydrogen in the mixture to produce the highest curve for chemical shift and, thus, can be eliminated. This leaves the chemical shift produced by the CH_2 protons present in the ketone form, the calculation of its relative area under the curve would, consequently, represent the concentration of the ketone in the tautomeric mixture of which the concertation is already known thus, obtaining the percentage of the ketone and the enol. Similarly, and using the same idea, the percentages can be calculated for all ketones/ enols.

Following this paper and to this day, NMR still remains the main method of calculation of the tautomeric percentages of ketones and enols making the need for a theoretical approach ever more needed. This is due to the fact that NMR machines are not readily accessible for the majority of chemists around the world, are expensive to obtain, and are expensive to run and maintain.

Many papers have been published which used NMR to determine tautomeric ratios of ketones and enols. Herein, I list two papers of specific importance and interest.

In a paper by Cook and Feltman [37] four compounds where used to test the solvent effect on the tautomerization ratio of keto/enols. The compounds were acetylacetone, dimedone, ethyl acetoacetate, and ethyl 4,4,4, -trifluoroacetoacetate (Figure 2.7) and the solvents were $CDCl_3$, DMSO, and Neat solution. The solvent effects on all four compounds were substantial; for example, for dimedone the enol % reported in $CDCl_3$, DMSO, and Neat were 7, 95, and 0 respectively.

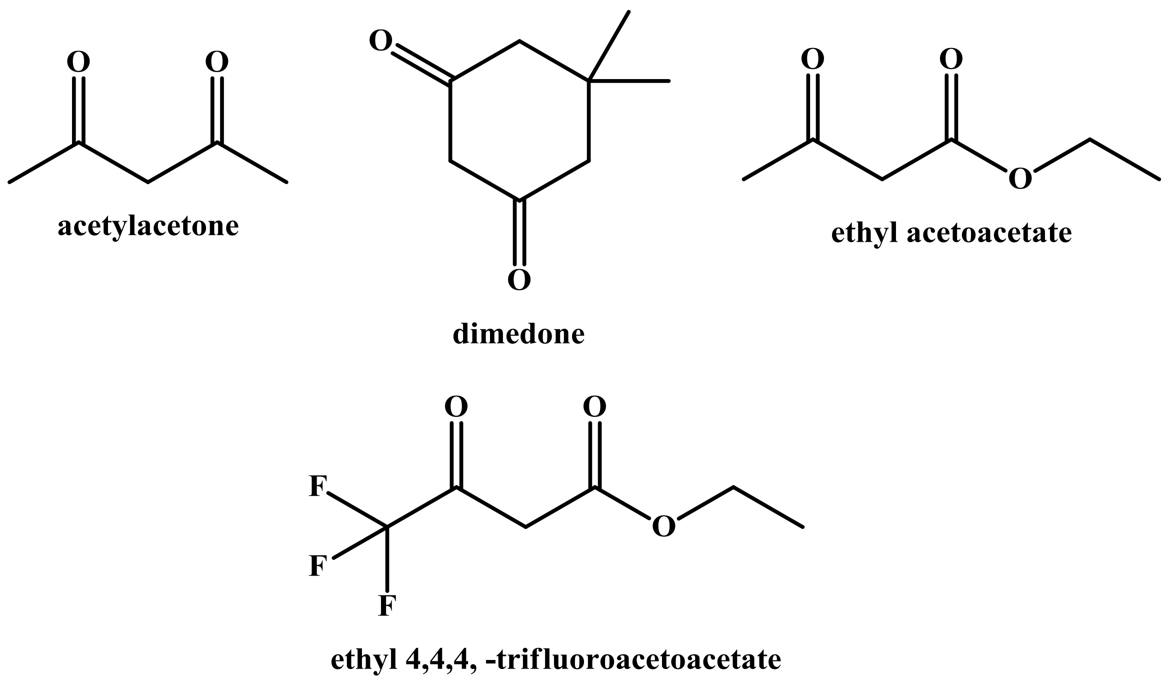


Figure 2.7: Chemical structures of compounds studied by Cook and Feltman

In a short paper by Marsh et al. [38] the proton NMR spectra of 2,4-pentanedione, 3-methyl-2,4-pentanedione, and 3-chloro-2,4-pentanedione (Figure 2.5) where recorded to study the effect of substituents on the keto-enol tautomerization equilibrium. They report that the chloro group leads to a more favoured enol while, on the contrary, the methyl group leads to a more favoured ketone. This is likely due to the electron withdrawing characteristic of the chloro substituent and the electron donating nature of the methyl group. This is probably due to stabilization of the conjugate base enolate by the chloro substituent and the destabilization of it by the methyl group.

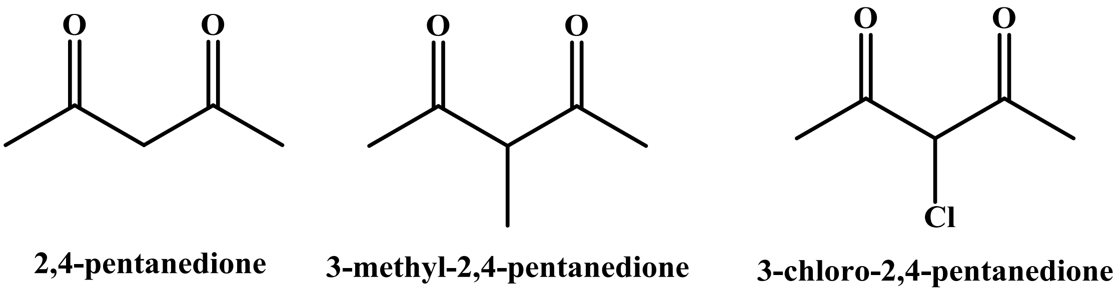


Figure 2.8: Chemical structures of compounds studied in the paper by Marsh et al.

2.1.5 Theoretical determination using computational methods

The main aim of this manuscript is to find a method which can predict with fair accuracy and affordable resources the keto/enol ratio. This is since currently the most commonly used method is NMR, which is not freely available to the majority of researchers and due to other reasons mentioned previously. A few researchers have taken this approach with marked success. Herein are papers which used theoretical methods to calculate the keto/enol ratio.

In a paper by Lien et al. [39] ab initio methods were used to study the keto-enol tautomerism of α-substituted acetaldehydes. Also, the team had previously calculated the ratios using G4 level of theory [40] The backbone of the molecule was $XH_2CCH=O$ (Figure 2.6) with X being H, BH2, CH_3, NH_2, OH, F, CN, NC, or Cl. Structures for ketones, enols, and stationary points were optimized using MP2(full)/6-31G* and MP2(full)/6-31G**. They found that at all levels of calculation, including G4 from their previous paper, the keto form was more thermodynamically stable.

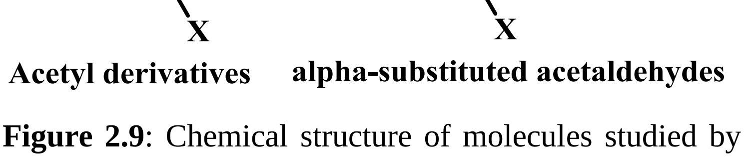


Figure 2.9: Chemical structure of molecules studied by Lien et al. where X is H, BH2, CH_3, NH_2, OH, F, CN, NC, or Cl

In a relatively recent paper by Acevedo, McFarkland, and McCann [41], gas phase predictions of 17 different quantum mechanical methods and eight basis sets was carried out for 7 different molecules. The molecules chosen are shown in Figure 2.7. The authors report that G4 and M06/6-31+G(d,p) yielded the most accurate results. Furthermore, those two methods were tested with three continuum solvent methods and six cavity models. The optimal combination reported by the authors was G4/PCM/UA0 and M06/6-31+G(d,p)/PCM/UA0 or UFF. This paper is the most encompassing of its kind in computational calculation of keto-enol tautomerism.

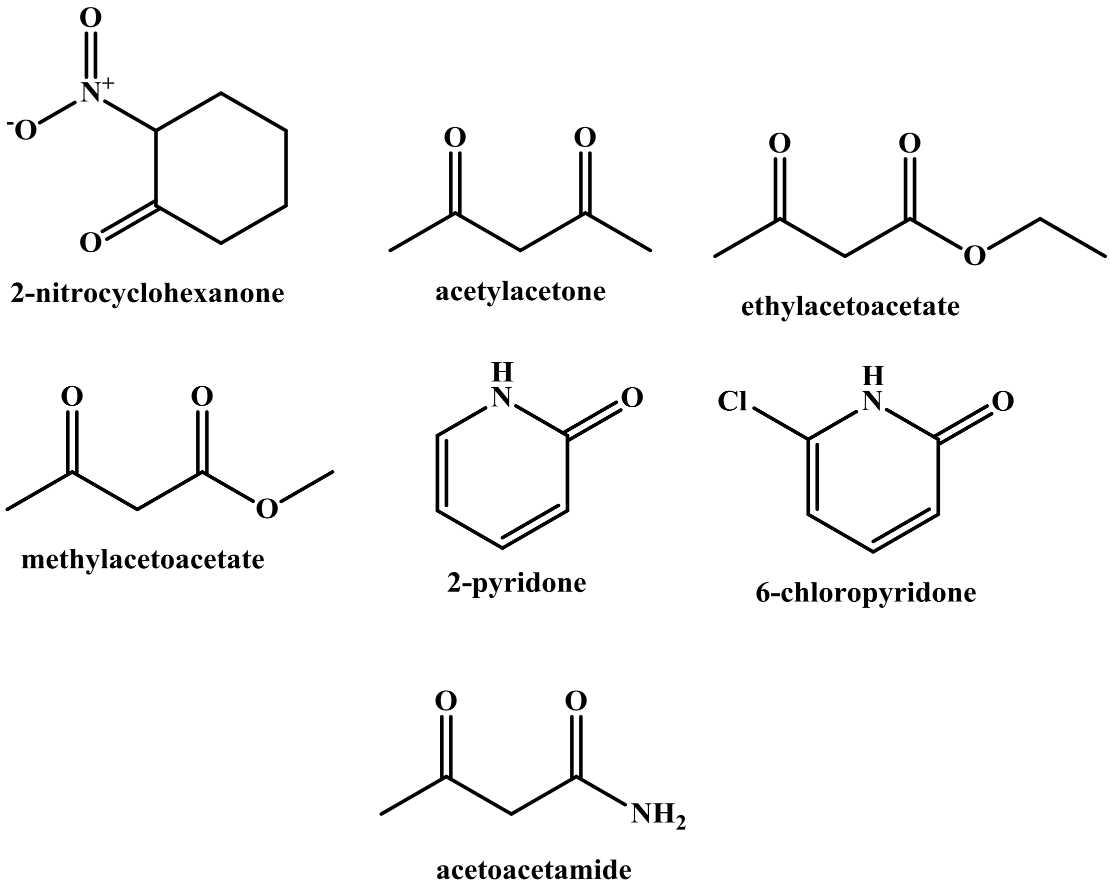


Figure 2.10: Chemical structures of molecules used in the Acevedo study

Other less applied approaches have been applied such as flash photolysis [42-44] and calorimetric determinations [45, 46]. A few references of value are included for further reading.

Chapter Three

Methodology

3. Methodology

3.1 Introduction

The main aim of this research was to find a reasonably accurate computational method which can predict the keto/enol ratio of a wide range of ketones/enols; i.e. small and simple in structure vs large and complex, in order to save resources and time by avoiding experimental lab measurements or NMR use, which in itself, is not readily available and is expensive to operate.

In order to provide a representative sample of molecules and their reported experimental keto/enol ratios, a deep literature scan was carried out using Google Scholar. Over 300 pieces of literature ranging from the 1950s to recently published ones were skimmed for reported tautomerization ratios and the experimental conditions under which they were obtained including the method, solvent, and temperature.

Furthermore, a scan of literature for computational methods used for numerous purposes that mainly revolve around the optimization of molecules found that the most commonly used methods were B3LYP, CAM-B3LYP, X3LYP, M05, M05-2X, M06, and M06-2X, thus, these methods were chosen for testing in this research. As is known, these methods are DFT hybrid methods, which provide fairly accurate results in molecule optimization when compared to *ab initio* methods, composite thermochemical methods or semiempirical quantum mechanical methods while saving time. This provides reasonable logic to their widespread application in the literature. The theory of these methods has been previously described in the introduction of this study.

Moreover, for each of the aforementioned methods chosen, 5 different basis sets were used;
6-31G(d,p), 6-31+G(d,p), 6-31++G(d,p), 6-311++G(d,p), and cc-pVDZ. These were, also, the most commonly used in the literature and were chosen. Since the aim was to find a reasonably cost-effective method, basis sets were limited to (d,p).

As is known, thus far, the method/basis set combinations are used optimize molecules in gas phase. This would not be expected to be representative of keto/enol ratios in solution. Hence, solvation of optimized molecules obtained from each method/basis set combination was calculated. However, a comparison of figures obtained from gas phase optimization with experimental values was also carried out.

The solvation phase of this research repeated the conditions (solvent, temperature) of the experiments reported in the literature. The default Gaussian-09 iefPCM model was used in solution-phase optimization. All cavity types available in Gaussian-09 were tested due to their effect on molecular energies and different atomic radii. These were: UFF, BONDI, PAULING, UA0, UAHF, and UAKS.

3.2 Software and hardware

Herein the software and hardware used in this study is listed.

3.2.1 Software

ArgusLab by Mark Thompson and Planaria Software LLC v4.0.1[47]

OpenBabel GUI © by Chris Morley v2.4.1 [48]

Gaussian 09 Revision A.02 [49]

Windows Office 2016 Professional plus v16.0.4266

AbleBits.com Ultimate Suite for Microsoft Excel v2016.4.484.1318

Notepad++ v7.7.1

Bulk Rename Utility TGRMN software v3.0.0.1

EndNote X7.0.1

Windows batch executables.

3.2.2 Hardware

Desktop 1: equipped with Windows 7 professional, CPU Intel core i7-6600, and 16GB of RAM

Desktop 2: equipped with Windows 7 professional, CPU Intel core i7-7700k, and 16GB of RAM

Laptop: equipped with Windows 7 professional, CPU Intel core i5-3210M, and 6GB of RAM

Virtual PCs: Amazon Webservices virtual instances size c5.2xlarge equipped with Windows Server 2019, CPU Xeon Platinum 8275CL, and 16GB of RAM

No graphics cards were used in the optimizations since their application is fairly new and limited to a few very expensive graphics cards which defeats the main aim of the study.

3.3 Application

Herein is reported a detailed step-by-step guide to the previously generally described methods: Firstly, upon obtaining the keto/enol ratio of a molecule from the literature, the molecular structure of the proposed tautomers was noted. Also, the experimental conditions that can be replicated, such as temperature, were also noted. A total of 52 molecules were chosen. The structures of the molecules are depicted in the figures at the end of this chapter.

Secondly, both the enol and ketone structures were drawn using ArgusLab and roughly optimized firstly using UFF then using PM3 to obtain an easier to optimize structure for input into Gaussian 09. A Gaussian input file was generated by ArgusLab for an HF/6-31G SP optimization.

Thirdly, the Gaussian input file was run and from it the output file provided the Z-matrix for the molecule. OpenBabel was used to generate a gzmat file to be used as the starting point for the optimization of each molecule.

Fourthly, each gzmat file was provided with the input line # 'Method/Basis Set' Freq Opt=(Z-matrix,MaxCycle=500,CalcFC) guess=indo SCF=noincfock integral(UltraFineGrid) GFINPUT IOP(6/7=3). Thus, each molecule had 35 different optimizations in gas phase since there are 7 methods and 5 basis sets. The output of this step provided the enthalpy, entropy, and Gibbs free energy for each molecule. These were obtained using personally written batch files and imported into excel sheets for calculation and analysis. The results obtained from this step provided comparison between gas-phase theoretically obtained ratios and experimentally obtained ratios from the literature.

Fifthly, the output file from step four was used to generate yet another gzmat file using OpenBabel, albeit this time for an optimized molecule. This gzmat file was modified and prepared for solvation-phase optimization. The input line used was # 'Method/Basis set' SP SCF=Tight SCRF=(iefPCM,Read,Solvent= 'Solvent'). Also, the solvation cavity was setup at the end of the gzmat file using radii= 'cavity'. Each molecule, prior to solvation, had been optimized 35 times for each of the methodology/ basis set combinations. Each of which provided an output file for the solvation phase optimization. Each molecule was solvated using the 6 aforementioned cavity types and in the appropriate solvent/s reported in the literature.

Step 5 provided solvation energies which were used to compare theoretically obtained ratios and experimentally obtained ratios.

Finally, taking into account gas-phase ratios and solvation-phase ratios, the best method which theoretically produced keto/enol ratios comparable to those obtained experimentally was chosen.

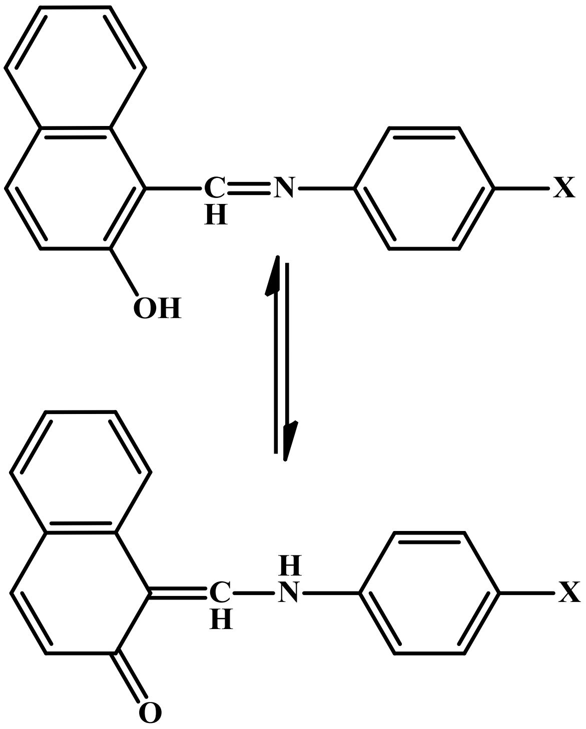
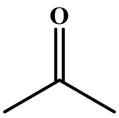
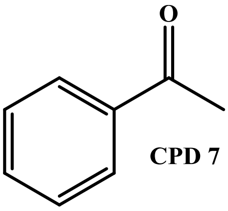


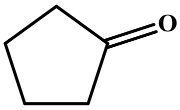
Figure 3.1: Structures of compounds (CPDs) 1-5 where X is: CPD 1= OH, CPD 2= OCH_3, CPD3= CH_3, CPD4= H, CPD 5= Cl.



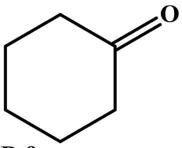
CPD 6



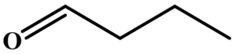
CPD 7



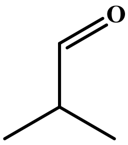
CPD 8



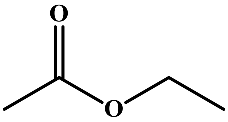
CPD 9



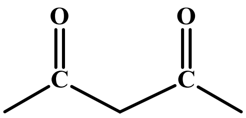
CPD 10



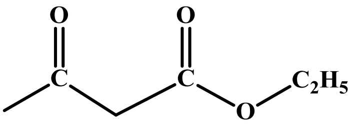
CPD 11



CPD 12

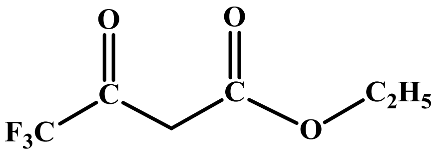


CPD 13

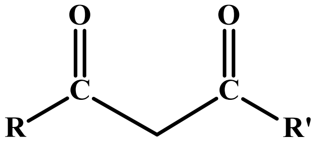


CPD 14

Figure 3.2: Structures of CPDs 6-14.

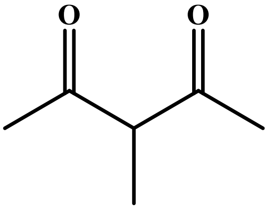


CPD 15

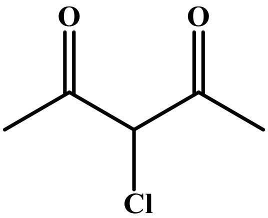


CPDs 16-40

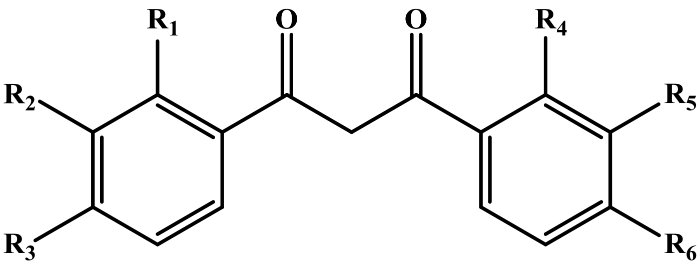
CPD 16: R,R'= C_2H_5
CPD 17: R,R'= n-C_4H_9
CPD 18: R,R'= n-C_5H_{11}
CPD 19: R,R'= i-C_3H_7
CPD 20: R,R'= i-C_4H_9
CPD 21: R,R'= t-C_4H_9
CPD 22: R,R'= CH_3, C_2H_5
CPD 23: R,R'= CH_3, i-C_5H_{11}
CPD 24: R,R'= CH_3, s-C_4H_9
CPD 25: R,R'= CH_3, i-C_3H_7
CPD 26: R,R'= CH_3, t-C_4H_9
CPD 27: R,R'= C_2H_5, n-C_3H_7
CPD 28: R,R'= C_2H_5, i-C_5H_{11}
CPD 29: R,R'= C_2H_5, i-C_4H_9
CPD 30: R,R'= C_2H_5, i-CH_3H_7
CPD 31: R,R'= C_2H_5, t-C_4H_9
CPD 32: R, R'= n-CH_3H_7, i-C_3H_9
CPD 33: R, R'= n-C_5H_{11}, i-C_4H_9
CPD 34: R, R'= C_6H_5, C_2H_5
CPD 35: R, R'= C_6H_5, n-C_3H_7
CPD 36: R, R'= C_6H_5, n-C_4H_9
CPD 37: R, R'= C_6H_5, i-C_3H_7
CPD 38: R, R'= C_6H_5, i-C_4H_9
CPD 39: R, R'= C_6H_5, i-C_5H_{11}
CPD 40: R, R'= C_6H_5, i-C_4H_9



CPD 41



CPD 42



Formula number	R^1	R^2	R^3	R^4	R^5	R^6
CPD 43	H	H	H	H	H	H
CPD 44	OMe	H	H	H	H	H
CPD 45	H	OMe	H	H	H	H
CPD 46	H	H	OMe	H	H	H
CPD 47	OMe	H	H	OMe	H	H
CPD 48	H	OMe	H	OMe	H	H
CPD 49	OMe	H	H	H	H	OMe
CPD 50	H	OMe	H	H	OMe	H
CPD 51	H	OMe	H	H	H	OMe
CPD 52	H	H	OMe	H	H	OMe

Figure 3.3: Structures of CPDs 15-52

Table 3.1: Enol percentages reported in the literature for the above compounds, and the solvents used where applicable.

CPD No.	Enol % reported in the literature	Solvent used (where applicable)
1	**41.7 [50]**	**Ethanol**
2	**44.1 [50]**	**Ethanol**
3	**44.1 [50]**	**Ethanol**
4	**48.3 [50]**	**Ethanol**
5	**47.6 [50]**	**Ethanol**
6	**6E-7 [51]**	**Neat**
7	**1.1E-6 [51]**	**Neat**
8	**1E-6 [51]**	**Neat**
9	**4E-5 [51]**	**Neat**
10	**5.5E-4 [51]**	**Neat**
11	**1.4E-2 [51]**	**Neat**
12	**0 [51]**	**Neat**
13	**86.0 [52]**	$CDCl_3$
13	**63.0 [52]**	**DMSO**
13	**80.0 [52]**	**Neat**
14	**3.0 [52]**	$CDCl_3$
14	**0 [52]**	**DMSO**
14	**8.0 [52]**	**Neat**
15	**85.0 [52]**	$CDCl_3$
15	**99.0 [52]**	**DMSO**
15	**89.0 [52]**	**Neat**
16	**80.0 [53]**	**Neat**
17	**91.7 [53]**	**Neat**
18	**91.7 [53]**	**Neat**
19	**95.8 [53]**	**Neat**
20	**95.3 [53]**	**Neat**
21	**98.0 [53]**	**Neat**
22	**82.1 [53]**	**Neat**

23	**91.6 [53]**	**Neat**
24	**93.4 [53]**	**Neat**
25	**91.6 [53]**	**Neat**
26	**93.7 [53]**	**Neat**
27	**85.2 [53]**	**Neat**
28	**88.5 [53]**	**Neat**
29	**89.2 [53]**	**Neat**
30	**90.8 [53]**	**Neat**
31	**93.4 [53]**	**Neat**
32	**93.7 [53]**	**Neat**
33	**94.6 [53]**	**Neat**
34	**93.9 [53]**	**Neat**
35	**95.9 [53]**	**Neat**
36	**95.6 [53]**	**Neat**
37	**97.0 [53]**	**Neat**
38	**97.4 [53]**	**Neat**
39	**96.8 [53]**	**Neat**
40	**98.1 [53]**	**Neat**
41	**20.5 [54]**	**CDCl3**
42	**92.9 [54]**	**CDCl3**
43	**94.0 [33]**	**DMSO**
43	**97.7 [33]**	**Acetone**
43	**97.8 [33]**	**CDCl3**
44	**90.2 [33]**	**DMSO**
44	**93.6 [33]**	**Acetone**
44	**91.6 [33]**	**CDCl3**
45	**94.6 [33]**	**DMSO**
45	**99.3 [33]**	**Acetone**
45	**97.3 [33]**	**CDCl3**
46	**93.7** [33]	**DMSO**
46	**97.3 [33]**	**Acetone**
46	**95.7 [33]**	**CDCl3**

47	**70.1 [33]**	**DMSO**
47	**87.1 [33]**	**Acetone**
47	**86.6 [33]**	**CDCl3**
48	**90.7 [33]**	**DMSO**
48	**95.3 [33]**	**Acetone**
48	**95.2 [33]**	**CDCl3**
49	**82.5 [33]**	**DMSO**
49	**92.0 [33]**	**Acetone**
49	**88.2 [33]**	**CDCl3**
50	**94.6 [33]**	**DMSO**
50	**97.8 [33]**	**Acetone**
50	**97.2 [33]**	**CDCl3**
51	**94.0 [33]**	**DMSO**
51	**96.4 [33]**	**Acetone**
51	**96.1 [33]**	**CDCl3**
52	**95.0 [33]**	**DMSO**
52	**96.7 [33]**	**Acetone**
52	**97.9 [33]**	**CDCl3**

Chapter Four

Results and Discussion

4 Results

ΔG for each of the molecules is calculated in accordance to equation 1.4 reported in the introduction section. Also ΔG for G calculated by the software was taken into account. In each table ΔG Calc. is ΔG obtained by the equation 1.4, ΔG Prog. is the ΔG obtained from the G reported by the software, absolute error is calculated using the following equation.

$$Erorr = \left| \frac{Theoretical - Experimental}{Experimental} x100\% \right|$$

Equation 4.1: Calculation of error of method employed

Outliers of convergence values vs experimental values were kept. In some convergences, the error was over 1000%, those were deemed as outliers and while they affect our vision of the level of theory or the basis set, they reflect the possibility of failure and not the accuracy of the level of theory or basis set. Also, molecules that the literature reported very low percentages of the enol form were mostly performed using the titration method. The titration method as mentioned earlier in the literature review section often exaggerate the enol content of molecules due to the inaccuracy of the method itself. The computational approach reported much lower concentrations; for example, for acetone the literature reported a percentage of 6E-7 while the computational method for B3LYP-6311++G, for example, reported a percentage of 4E-10. This results in the absolute error according to the equation above to be over 100 thousand %. This, of course, means that the discrepancy in the percentage between the literature and the computation leads to treating the absolute error as an outlier. The same applies for all molecules with low concentrations. The absolute error with outliers removed is a better reflection of the accuracy of the method.

The full tables are listed in the appendices.

4.1 Primary objective

Herein are reported the results of the primary objectives. Firstly, a comparison between the literature values and the results obtained from the gas phase are reported. This is simplified to a comparison between different functionals and their basis sets in tables. Also, the average absolute error with and without outliers is reported in the tables. Moreover, the number of failed convergences and outliers is also included in the tables. The average absolute error without outliers is taken as an indicator of the accuracy of the method in tandem with the number of failed convergences. Secondly, the results of the solvation phase are reported in a similar fashion to the gas phase results and are taken as the final word in which functional/basis set combination is the optimal one.

4.1 Gas phase results

The first optimization was performed in gas phase then the optimized molecule from the gas phase were solvated in the appropriate solvent according to the literature.

4.1.1 B3LYP

Basis set	6311++G (d,p)	631++G (d,p)	631+G (d,p)	631G (d,p)	cc-pVDZ
Average absolute error with outliers	1.08E7%	6.78E6%	4.39E4%	9.83E5%	3.22E5%
Average absolute error without outliers	14.09%	14.81%	12.61%	12.56%	12.63%
Number of failed convergences	9	10	9	3	5
Number of outliers	10	10	8	8	7

Table 4.1 Results of B3LYP in gas phase showing average absolute error for every basis set.

A quick look at the results of B3LYP shows that basis sets with less split-valence and lower polarization such as 631+G or 631G show better results. However, 631G appears to be the best basis set for B3LYP for two reasons. Firstly, it produced the lowest average absolute error when outliers removed. Secondly, the number of failed convergences is significantly lower than other basis sets. However, while 12.56% average absolute error is somewhat acceptable, it is, though, far from optimal. In addition, the number of molecules that failed to converge is 3, which is around 6% of all molecules. A success rate of 94% is attractive.

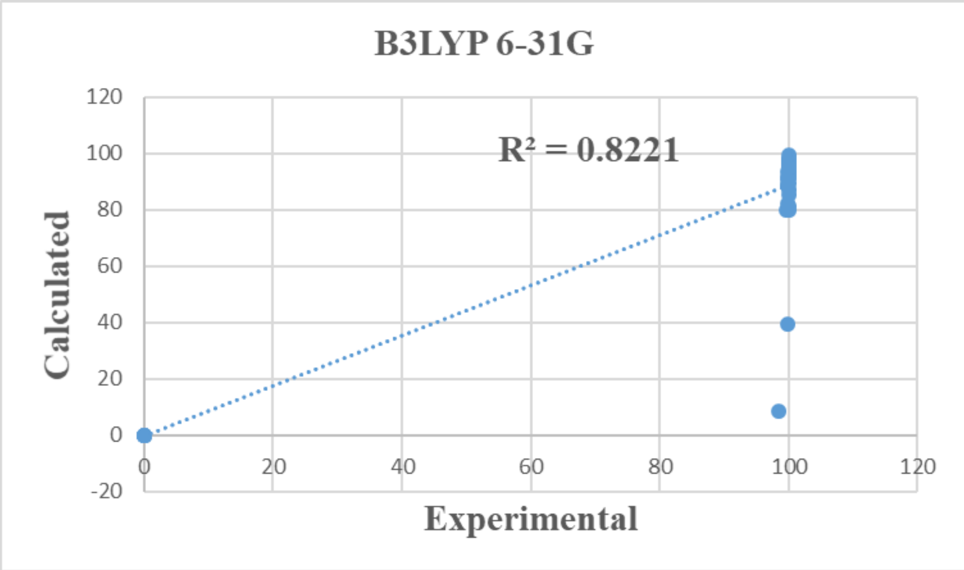


Figure 4.1: Experimental vs calculated values showing R^2 values for B3LYP 6-31G

4.1.2 CAM-B3LYP

Basis set	6-311++G (d,p)	6-31++G (d,p)	6-31+G (d,p)	6-31G (d,p)	cc-pVDZ
Average absolute error with outliers	9.98E5%	6.32E8%	9.29E5%	3.22E5%	5.81E5%
Average absolute error without outliers	15.23%	14.82%	13.16%	12.63%	14.05%
Number of failed convergences	10	7	4	5	3
Number of outliers	8	9	8	8	8

Table 4.2 Results of CAM-B3LYP in gas phase showing average absolute error for every basis set.

The results of CAM-B3LYP are somewhat disappointing. This echoes correspondence with one of the authors of the benchmarking paper (reference 37) who stated that CAM-B3LYP would produce good results out of sheer luck and coincidence, and that the long range the CAM-B3LYP offers over the normal B3LYP would be expected to produce poorer results. Four out of five basis sets failed to produce an acceptable average absolute error value. In turn, and similar to B3LYP, 6-31G produced the least average absolute error with a value of 12.63% which is nearly identical to the value produced by B3LYP 6-

31G. The number of molecules that failed to converge for CAM-B3LYP 631G is around 10%, since there are 52 molecules. This gives this functional/basis set combination a success rate of 90%. This is lower than what was produced by B3LYP-6-31G. So far, the combination of B3LYP-6-31G is the best in gas phase.

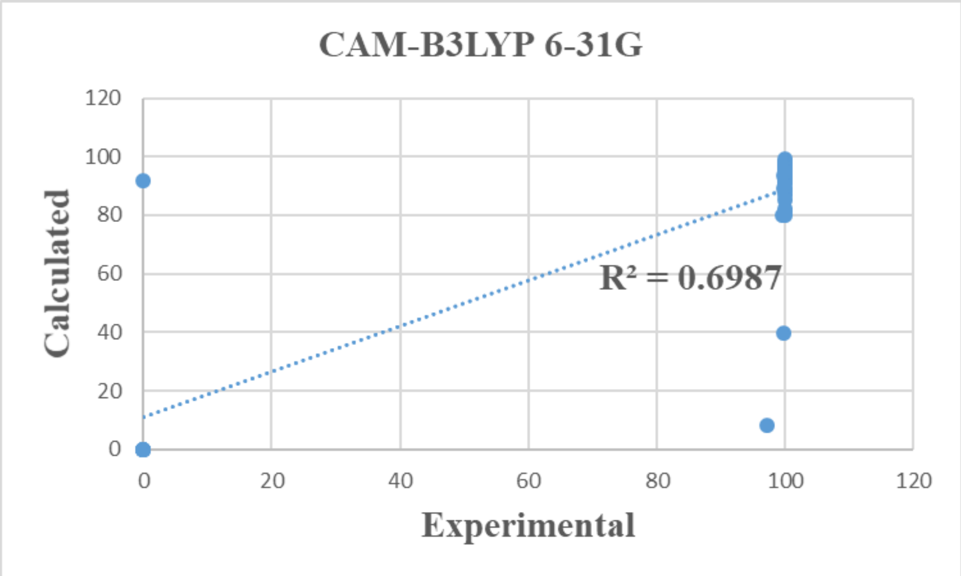


Figure 4.2: Experimental vs calculated values showing R^2 values for CAM-B3LYP 6-31G

4.1.3 X3LYP

Basis set	6-311++G (d,p)	6-31++G (d,p)	6-31+G (d,p)	6-31G (d,p)	cc-pVDZ
Average absolute error with outliers	1.67E6%	1.71E6%	2.99E2%	1.05E4%	2.78E3%
Average absolute error without outliers	13.80%	14.21%	13.74%	15.03%	12.84%
Number of failed convergences	15	14	13	8	4
Number of outliers	8	9	6	8	8

Table 4.3 Results of X3LYP in gas phase showing average absolute error for every basis set.

X3LYP is a newer modified version of the B3LYP functional devised by Xu and Goddard in 2004 [17], nearly 10 years after Becke et al. devised the B3LYP functional [13]. The X in X3LYP here stands for extended, i.e. the functional is meant to work at longer ranges and avoid Gaussian decay, like the previously reported CAM-B3LYP functional. Xu et al. claimed that this extension to the existing B3LYP functional should improve the accuracy for hydrogen bonding, heat of formation, and total atomic energies. In their paper they also state that B3LYP is the most popular and accurate method available at the time.

However, from our calculations on ketones and enols we see that X3LYP performs, in fact, more poorly than B3LYP. All basis sets except for cc-pVDZ performed poorly in our calculations. In the previous B3LYP and CAM-B3LYP, 6-31G performed the best, albeit not well enough, however in X3LYP this was not the case. It is difficult to offer explanations as to why this happened, it is perhaps speculative to attempt to explain the results. The results of the X3LYP-cc-pVDZ combination are similar to those reported by the best basis sets in CAM-B3LYP and B3LYP with an average absolute error of 12.84% and 4 failed convergences. However, B3LYP 6-31G still remains the best combination thus far.

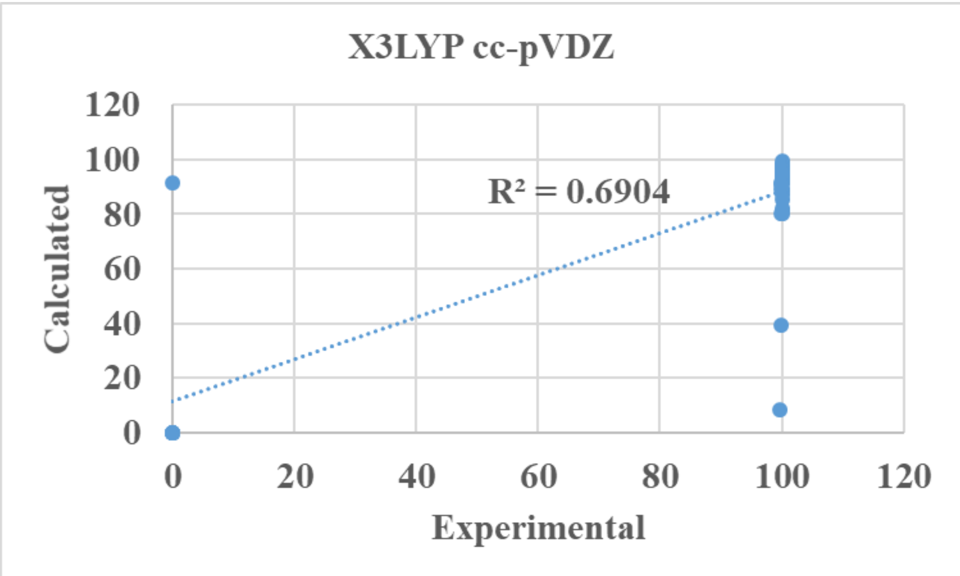


Figure 4.3: Experimental vs calculated values showing R^2 values for X3LYP cc-pVDZ

4.1.4 M05

Basis set	6-311++G (d,p)	6-31++G (d,p)	6-31+G (d,p)	6-31G (d,p)	cc-pVDZ
Average absolute error with outliers	4.00E5	6.95E8	3.46E8	2.56E5	8.19E5
Average absolute error without outliers	22.97%	18.24%	14.27%	13.56%	18.89%
Number of failed convergences	13	20	27	19	20
Number of outliers	8	11	11	8	8

Table 4.4 Results of M05 in gas phase showing average absolute error for every basis set.

Thus far, M05 delivered the poorest results of the functionals. It was designed by Zhao et al. in 2005 [18] and compared it to the best functional at the time PW6B95. This comparison, they claim in the paper, showed that M05 performs 1.4 times better. The main aim behind the design of M05 is to incorporate kinetic-energy density in the exchange and correlational functionals. The method is meant to be applicable to organometallic, inorganometallic, and non-metallic bonding, as well as, theromochemical kinetics. However, and while this method is much newer than the best performer thus far in this study, B3LYP, it appears that M05 is not the functional of choice for the determination of keto/enol tautomerism. As it is seen in the table, the average absolute error is high in all basis sets. Also, the number of failed convergences is alarmingly high when compared to aforementioned methods. As is the case with X3LYP, one cannot put their finger on a clear reason behind this failure. One can only conclude that this is not the method of choice for the prediction of keto/enol tautomerism. It should be noted that this part is still comparing the gas phase results while the literature reported solvated results. Perhaps M05 fairs better in predicting the tautomerism ratio in solvents.

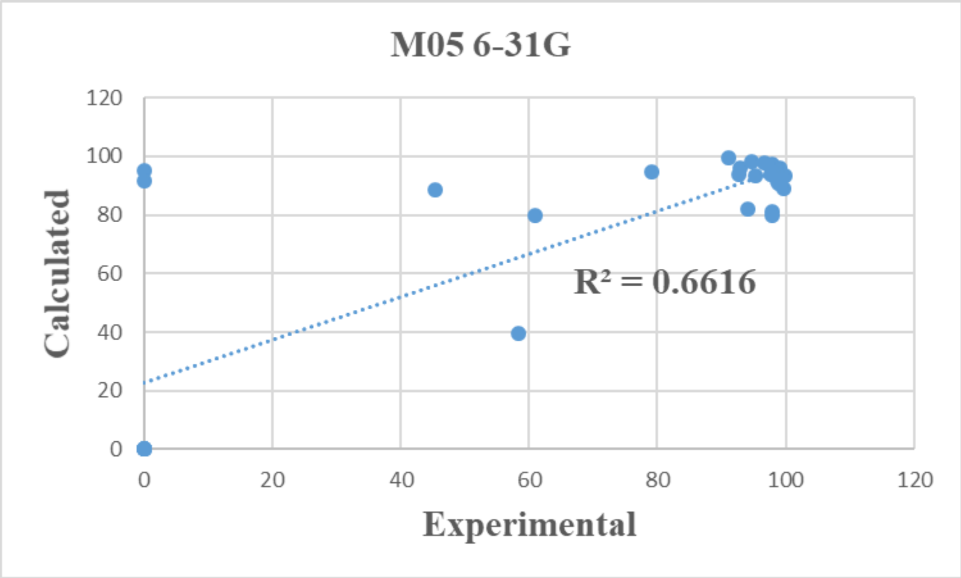


Figure 4.4: Experimental vs calculated values showing R^2 values for M05 6-31G

4.1.5 M05-2X

Basis set	6-311++G (d,p)	6-31++G (d,p)	6-31+G (d,p)	6-31G (d,p)	cc-pVDZ
Average absolute error with outliers	1.79E3%	4.47E5%	1.44E3%	2.79E3%	1.99E3%
Average absolute error without outliers	15.70%	18.34%	13.61%	12.41%	16.75%
Number of failed convergences	13	20	16	14	11
Number of outliers	8	10	8	8	8

Table 4.5 Results of M05-2X in gas phase showing average absolute error for every basis set.

M05-2X showed an improvement over M05 but still it is not good enough, speaking for the gas phase that is. In its inception, in a publication by Zhao et al.[19], the authors claimed that it had the best performance for thermochemical kinetics, noncovalent interactions, and alkyl bond dissociation energies. This method excluded metals in contrast to the original M05. While the keto/enol tautomerism does not rely on covalent interactions, has dissociation of bonds, and is heavily reliant on thermochemical kinetics, M05-2X failed to provide a reliable functional/basis set combination in this study, at least for the gas phase. Although 6-31G exhibited low average absolute error, it failed to achieve convergence in 14 instances. This may be related to the calculation conditions and the limited number of cycles. Though the same conditions were applied to other functionals, most of them produced better results in the gas phase. M05-2X was an improvement over M05, but using it is ill-advised for ketones and enols.

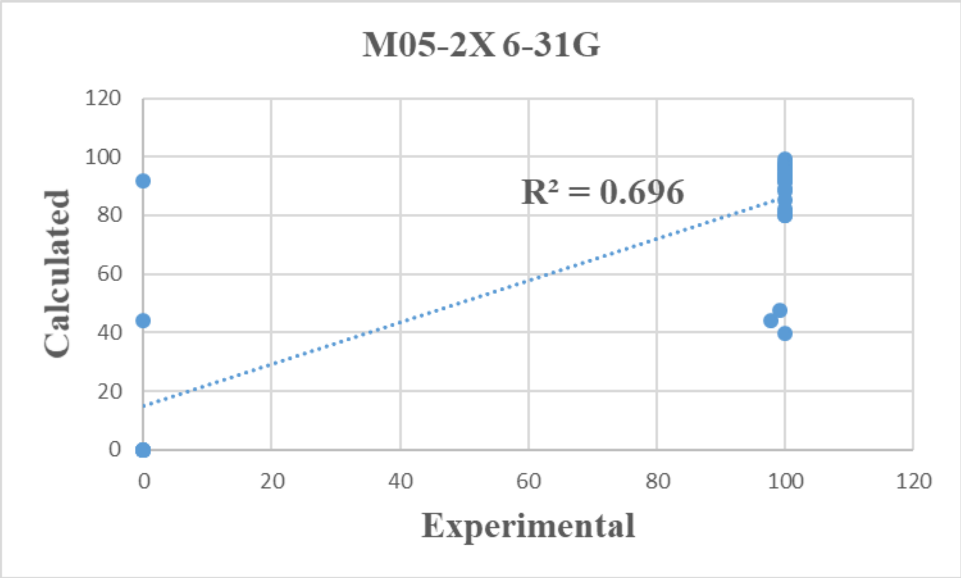


Figure 4.5: Experimental vs calculated values showing R^2 values for M05-2X 6-31G

4.1.6 M06

Basis set	6-311++G (d,p)	6-31++G (d,p)	6-31+G (d,p)	6-31G (d,p)	cc-pVDZ
Average absolute error with outliers	2.40E8%	1.05E4%	8.89E7%	2.83E4%	1.22E4%
Average absolute error without outliers	17.19%	12.33%	16.02%	16.05%	18.18%
Number of failed convergences	23	21	19	16	19
Number of outliers	8	8	8	7	8

Table 4.6 Results of M06 in gas phase showing average absolute error for every basis set.

Zhao et al., the producers of the M05 and M05-2X functionals in 2005, developed a series of M06 functionals 3 years later [14]. The new functionals, including M06, M06-2X, M06-L, and others, meant to have improvements over the older functionals in areas such as thermochemical dynamics, kinetics, non-covalent interactions, and other properties. However, in this study M06 appears to perform similarly to M05 with slightly better figures. They are, however, still poor figures when compared to B3LYP, CAM-B3LYP, and even X3LYP. The number of convergence failures is high making the functional unreliable, and the average absolute error is high making it inaccurate. The study (reference 17) concluded that M06 and M06-2X are the best functionals at the time. In gas phase, at least, they are not recommended for studying keto/enol tautomerism.

4.1.7 M06-2X

Basis set	6311++G (d,p)	631++G (d,p)	631+G (d,p)	631G (d,p)	cc-pVDZ
Average absolute error with outliers	5.48E6%	5.10E6%	1.26E7%	4.13E3%	1.07E4%
Average absolute error without outliers	12.03%	14.92%	17.25%	14.44%	15.35%
Number of failed convergences	14	13	15	17	10
Number of outliers	8	9	9	6	8

Table 4.7 Results of M06-2X in gas phase showing average absolute error for every basis set.

The results of M06-2X are better than M06, in the same fashion that M05-2X was better than M05. This agrees with what Zhao et al. claimed in their paper. However, the results are still unsatisfactory for keto/enol tautomerism calculation. While 6311++ exhibited the least average absolute error with outliers removed, it failed to achieve convergence for 14 molecules making it unreliable. In the gas phase, B3LYP/6-31G provided the best reliability and a fair level of accuracy with a low average absolute error.

4.2 Solvation Results

Following gas phase convergence, gzmat files were obtained from the output of the gas phase calculation. Obviously, the molecules that failed to converge in the gas phase provided no means for comparison. The solvation phase calculations were single point, PCM calculations, and not freq calculations, thus, enthalpy and entropy were not part of the calculations. The solvation phase calculations were carried out as follows:

$$(Enol\ \Delta G_{Solv} - \left(-Enol\ \Delta G_{gas}\right) x\ 627.5095$$

Equation 4.2: Calculation of ΔG difference between gas phase and solvated phase converted to Calories.

The above calculation was inspired by Lewars' [55] The same equation was applied to ketone results. This produced ΔG differences between solvated molecules and gas phase molecules for both ketones and enols. The difference between the two resulting ΔGs was calculated then input into Arrhenius' equation (equation 1.5).

However, since the literature reported results for neat solutions in some cases, the calculation of solvation was not possible as previously mentioned. Hence, herein, are reported the solvation phase results for each functional and its basis sets for each solvation cavity and a comparison of the average absolute error. Molecules that failed in the gas phase were omitted, outliers were kept but were not included in the average absolute error calculations as was done for the gas phase results.

4.2.1 B3LYP Solvation Results

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ	Average absolute error for cavity
UFF	21.4%	30.4%	14%	26.1%	17.2%	21.82%
UAKS	21.4%	34.0%	16.0%	30.0%	20.0%	24.28%
UA0	25.8%	38.0%	17.0%	35%	24.3%	28.02%
Bondi	20.6%	19.4%	13.9%	12.5%	11.1%	15.50%
Pauling	22.5%	20.6%	15.1%	14.2%	13.3%	17.14%
UAHF	22.8%	23.3%	15.1%	14.8%	14.3%	18.06%

Table 4.8 Average absolute error for each basis set and cavity for solvated molecules using B3LYP functional

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ
UFF	7	5	1	1	1
UAKS	7	5	1	1	1
UA0	7	5	1	1	1
Bondi	7	7	1	1	1
Pauling	7	7	1	1	1
UAHF	7	5	1	1	1

Table 4.9: Number of outliers for each basis set and cavity for Table 4.8

4.2.2 CAM-B3LYP Solvation Results

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ	Average absolute error for cavity
UFF	19.4%	12.7%	13.7%	16.8%	17.9%	16.1%
UAKS	20.0%	13.6%	15.3%	14.5%	16.2%	15.9%
UA0	22.1%	14.9%	15.4%	21.6%	29.1%	20.6%
Bondi	18.5%	12.2%	14.2%	12.5%	14.3%	14.3%
Pauling	19.8%	13.4%	15.1%	14.0%	15.4%	15.5%
UAHF	19.8%	13.6%	15.1%	14.4%	16.2%	15.8%

Table 4.10: Average absolute error for each basis set and cavity for solvated molecules using B3LYP functional

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ
UFF	1	3	1	1	1
UAKS	1	3	1	1	1
UA0	1	3	1	1	1
Bondi	1	3	1	1	1
Pauling	1	3	1	1	1
UAHF	1	3	1	1	1

Table 4.11: Number of outliers for each basis set and cavity for Table 4.10

4.2.3 X3LYP Solvation Results

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ	Average absolute error for cavity
UFF	14.4%	15.9%	16.4%	22.6%	17.8%	17.4%
UAKS	14.4%	15.9%	16.4%	22.6%	17.8%	17.4%
UA0	14.4%	15.9%	16.4%	22.6%	17.8%	17.4%
Bondi	14.5%	12.3%	13.4%	12.8%	11.5%	12.9%
Pauling	14.3%	14.6%	15.1%	14.5%	13.6%	14.4%
UAHF	14.4%	15.9%	16.4%	16.4%	17.8%	16.2%

Table 4.12: Average absolute error for each basis set and cavity for solvated molecules using X3LYP functional

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ
UFF	4	3	1	1	1
UAKS	4	3	1	1	1
UA0	4	3	1	1	1
Bondi	3	3	1	1	1
Pauling	3	3	1	1	1
UAHF	4	3	1	1	1

Table 4.13: Number of outliers for each basis set and cavity for Table 4.12

4.2.4 M05 Solvation Results

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ	Average absolute error for cavity
UFF	15.0%	14.0%	36.2%	15.7%	19.9%	20.2%
UAKS	15.0%	14.0%	36.2%	15.7%	19.9%	20.2%
UA0	21.6%	17.2%	69.5%	23.7%	25.6%	31.5%
Bondi	10.9%	12.6%	18.7%	6.4%	16.8%	13.1%
Pauling	12.7%	14.0%	19.1%	7.5%	19.3%	14.5%
UAHF	11.2%	14.3%	16%	16.0%	17.3%	14.7%

Table 4.14: Average absolute error for each basis set and cavity for solvated molecules using M05 functional

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ
UFF	0	3	3	0	0
UAKS	0	3	3	0	0
UA0	0	3	3	0	0
Bondi	0	3	3	0	0
Pauling	0	3	3	0	0
UAHF	0	3	3	0	0

Table 4.15: Number of outliers for each basis set and cavity for Table 4.14

4.2.5 M05-2X Solvation Results

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ	Average absolute error for cavity
UFF	2.1%	17.0%	6.3%	9.4%	10.3%	9.0%
UAKS	4.3%	16.8%	9.2%	8.7%	14.1%	10.6%
UA0	2.2%	17.5%	Failed	Failed	Failed	-
Bondi	4.1%	15.2%	8.5%	6.6%	12.9%	9.5%
Pauling	4.3%	16.3%	6.6%	8.1%	7.2%	8.5%
UAHF	4.2%	16.8%	9.2%	9.2%	14.1%	10.7%

Table 4.16: Average absolute error for each basis set and cavity for solvated molecules using M05-2X functional

Basis Set Solvation Cavity	6-311++G	6-31++G	6-31+G	6-31G	cc-pVDZ
UFF	0	3	0	0	0
UAKS	0	3	0	0	0
UA0	0	4	Failed	Failed	Failed
Bondi	0	3	0	0	0
Pauling	0	3	0	0	0
UAHF	0	3	0	0	0

Table 4.17: Number of outliers for each basis set and cavity for Table 4.16

4.2.5 M06 Solvation Results and M06-2X Solvation Results

Due to the poor performance of the functionals in the gas phase solvation results were too poor to report. Each cavity had more outliers than results and most of the solvated molecules either failed in the gas phase and no comparison was possible or reported errors over 80%.

The solvation results reported by the functionals and their basis sets in the proceeding tables show that when it comes to choice of cavity Bondi parameters were the best. Though M05 and M05-2X appear to have had the best performance in the solvation phase the results of the gas phase were poor. This meant that the results of the solvation phase were for fewer molecules than other functionals and are not representative. However, M05-2X/6-311++G (d,p) with a Bondi cavity is a good choice for solvation still. B3LYP performed modestly in the solvation phase but the sample of compounds that were solvated was much higher than the rest of the functionals due to its best performance in the gas phase. This leads us to the conclusion that the B3LYP/6-31G (d,p) with a Bondi cavity is the best choice for optimizing a ketone or enol from scratch to solvation in order to obtain the keto/enol ratio.

5. Summary, conclusion and further research

This study conducted on 52 molecules with reported experimental keto/enol ratios aimed to find the optimal functional/basis set combination from 7 of the most commonly used functionals in the literature. The basis sets were kept simple to find a combination that was quick. The study managed to achieve its aim, reporting that B3LYP/6-31G (d,p) was the best choice for finding the keto/enol ratio of a given compound. The best solvation cavity for this was Bondi for whichever function/basis set combination choice. The optimal functional reported by the study was the most commonly used one in the literature. However, no comparison on a large number of molecules for the aim of finding the keto/enol ratio had been conducted before. Thus, and while it was the most commonly reported, this study provides evidence and reassurance for its use in this kind of test.

Further research needs to be conducted; the data of this study provides means to find a statistical correlation that is representative for all the functionals and basis sets vs time or accuracy. Research can be carried to test whether an optimal solvent can be found that can be used to solvate the compounds reported as neat solutions. Also, regarding compounds, statistical correlation can be found between the size of the molecule, how many halogen groups are present, rings, etc… and the time needed for convergence. Most importantly, research can be conducted to compare the optimal functional found by this study with other functionals.

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Appendices

Appendices

Gas Phase Results

1.1 B3LYP gas phase

1.1.1 B3LYP 6-311++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.64589124	-0.645707276	74.8545098	74.848661	41.7	44.29%	44.29%
2 ethanol	-47202.5006	-47202.50078	N/A	N/A	44.1	N/A	N/A
3 ethanol	0.274590131	0.274221652	38.6093123	38.6240644	44.1	14.22%	14.18%
4 ethanol	0.004112969	0.003765057	49.8263374	49.8410272	48.3	3.06%	3.09%
5 ethanol	N/A	N/A	N/A	N/A	47.6	N/A	N/A
6	15.48400072	15.48442442	4.391E-10	4.38789E-10	6E-7	136543.13%	136639.98%
7	15.44049275	15.44049876	4.726E-10	4.72579E-10	1.1E-6	232654.97%	232665.32%
8	14.42425477	14.42456088	2.63E-9	2.62821E-9	1E-6	37922.81%	37948.71%
9	12.19358931	12.19313709	1.138E-7	1.13867E-7	4E-5	35049.38%	35028.70%
10	9.99201372	9.991833768	4.687E-6	4.68859E-6	5.5E-4	11634.59%	11630.61%
11	7.110836084	7.111565164	0.0006085	0.000607717	1.4E-2	2200.74%	2203.70%
12	15.44049275	31.4940743	7.942E-22	7.92977E-22	0	0	0
13 $CDCl_3$	-4.596505118	-4.595879578	99.957508	99.95746353	86.0	13.96%	13.96%
13 DMSO	-4.596505118	-4.595879578	99.957508	99.95746353	63.0	36.97%	36.97%

13	-4.596505118	-4.595879578	99.957508	99.95746353	80.0	19.97%	19.97%
14 $CDCl_3$	-1.957845679	-1.957202131	96.465701	96.46199322	3.0	96.89%	96.89%
14 DMSO	-1.957845679	-1.957202131	96.465701	96.46199322	0	0	0
14	-1.957845679	-1.957202131	96.465701	96.46199322	8.0	91.71%	91.71%
15 $CDCl_3$	-2.619568733	-2.619852163	98.815904	98.81646422	85.0	13.98%	13.98%
15 DMSO	-2.619568733	-2.619852163	98.815904	98.81646422	99.0	0.19%	0.19%
15	-2.619568733	-2.619852163	98.815904	98.81646422	89.0	9.93%	9.93%
16	-4.590542118	-4.590231993	99.957079	99.95705603	80.0	19.97%	19.97%
17	-2.484490791	-2.48493762	98.51697	98.51807201	91.7	6.92%	6.92%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-5.609743733	-5.609307421	99.992322	99.99231633	95.8	4.19%	4.19%
20	-5.20555789	-5.205818812	99.984806	99.98481226	95.3	4.69%	4.69%
21	6.7599639	6.759532334	0.0011005	0.00110132	98.0	8904943.16%	8898312.81%
22	-4.313905483	-4.314127813	99.931534	99.93155962	82.1	17.84%	17.84%
23	-3.308103322	-3.307602574	99.626836	99.62652142	91.6	8.06%	8.06%
24	N/A	N/A	N/A	N/A	93.4	N/A	N/A
25	-5.225470218	-5.225271607	99.985308	99.98530307	91.6	8.39%	8.39%
26	7.215452158	7.215104231	0.0005099	0.000510219	93.7	18376052.19%	18364563.02%
27	-4.92139175	-4.921557	99.975448	99.97545534	85.2	14.78%	14.78%
28	-3.81706332	-3.8171403	99.841687	99.84170781	88.5	11.36%	11.36%

29	-3.67161193	-3.6715581	99.797692	99.79767401	89.2	10.62%	10.62%
30	N/A	N/A	N/A	N/A	90.8	N/A	N/A
31	-3.5604079	-3.5604889	99.755995	99.75602851	93.4	6.37%	6.37%
32	-4.6955474	-4.69565359	99.964051	99.96405765	93.7	6.27%	6.27%
33	-3.2963593	-3.2963074	99.619389	99.61935563	94.6	5.04%	5.04%
34	-6.282074	-6.2819976	99.997533	99.99753296	93.9	6.10%	6.10%
35	-4.0991796	-4.09889205	99.901634	99.90158611	95.9	4.01%	4.01%
36	-4.2197936	-4.21937388	99.919748	99.91969135	95.6	4.32%	4.32%
37	-4.1571542	-4.15725044	99.910801	99.91081518	97.0	2.91%	2.91%
38	-5.2960494	-5.29555267	99.986959	99.98694782	97.4	2.59%	2.59%
39	-4.2752827	-4.27584973	99.926922	99.92699219	96.8	3.13%	3.13%
40	-4.6157594	-4.61595988	99.958867	99.95888135	98.1	1.86%	1.86%
41 $CDCl_3$	-5.3591975	-5.35955864	99.988278	99.98828504	40.5	59.50%	59.50%
42 $CDCl_3$	-2.784603	-2.78488716	99.101356	99.10178307	92.6	6.56%	6.56%
43 DMSO	-5.28151179	-5.28112	99.93712	99.93711971	94.0	5.94%	5.94%
43 Acetone	-5.28151179	-5.28112	99.93712	99.93711971	97.7	2.24%	2.24%
43 $CDCl_3$	-5.28151179	-5.28112	99.93712	99.93711971	97.8	2.14%	2.14%
44 DMSO	-6.67202968	-6.671681	99.986635	99.9866258	90.2	9.79%	9.79%
44 Acetone	-6.67202968	-6.671681	99.986635	99.9866258	93.6	6.39%	6.39%
44 $CDCl_3$	-6.67202968	-6.671681	99.986635	99.9866258	91.6	8.39%	8.39%

45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A
45 $CDCl_3$	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 DMSO	11.32088957	11.3208989	4.9681E-7	4.968E-7	93.7	18860328798.37%	18860708434.62%
46 Acetone	11.32088957	11.3208989	4.9681E-7	4.968E-7	97.3	19584951893.72%	19585346115.78%
46 $CDCl_3$	11.32088957	11.3208989	4.9681E-7	4.968E-7	95.7	19262897184.68%	19263284924.15%
47 DMSO	-6.75610332	-6.7563948	99.9988923	99.9988928	70.1	29.90%	29.90%
47 Acetone	-6.75610332	-6.7563948	99.9988923	99.9988928	87.1	12.90%	12.90%
47 $CDCl_3$	-6.75610332	-6.7563948	99.9988923	99.9988928	86.6	13.40%	13.40%
48 DMSO	10.18516178	10.1851067	3.3825E-6	3.3828E-6	90.7	2681448532.67%	2681210731.26%
48 Acetone	10.18516178	10.1851067	3.3825E-6	3.3828E-6	95.3	2817442619.88%	2817192757.99%
48 $CDCl_3$	10.18516178	10.1851067	3.3825E-6	3.3828E-6	95.2	2814486226.68%	2814236626.97%
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92.0	N/A	N/A
49 $CDCl_3$	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-4.95177116	-4.9516775	99.9766761	99.9766725	94.6	5.38%	5.38%
50 Acetone	-4.95177116	-4.9516775	99.9766761	99.9766725	97.8	2.18%	2.18%
50 $CDCl_3$	-4.95177116	-4.9516775	99.9766761	99.9766725	97.2	2.78%	2.78%
51 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A

51 $CDCl_3$	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95.0	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 $CDCl_3$	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.08E7%	1.08E7%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.09%	14.09%

Table 1.1: Convergence results from B3LYP-6311++ gas phase and how it compares to experimental data.

1.1.2 B3LYP 6-31++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.56450227	-0.5647586	72.1799871	72.188678	41.7	42.23%	42.23%
2 ethanol	-47190.4802	-47190.48	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.24103606	-0.2409636	60.0390878	60.0361537	44.1	26.55%	26.54%
4 ethanol	-0.16181847	-0.1618975	56.7903051	56.7935786	48.3	14.95%	14.96%
5 ethanol	-0.48800654	-0.4882024	69.5129471	69.5199566	47.6	31.52%	31.53%
6	16.358652	16.3585452	1.0023E-10	1.0025E-10	6E-7	598523.17%	598403.74%
7	15.9738247	15.9732543	1.9199E-10	1.9218E-10	1.1E-6	572846.51%	572280.06%
8	14.91027316	14.9102532	1.1572E-9	1.1572E-9	1E-6	86315.49%	86315.49%

9	12.62519831	12.6254911	5.4889E-8	5.4862E-8	4E-5	72774.35%	72810.21%
10	10.5466863	10.5459247	1.8368E-6	1.8392E-6	5.5E-4	29843.38%	29804.31%
11	7.249006388	7.24898974	0.00048183	0.00048184	1.4E-2	2805.59%	2805.53%
12	31.90034052	31.9007005	3.9927E-22	3.9903E-22	0	0%	0%
13 CDCl3	-4.98219306	-4.9817979	99.977844	99.9778292	86.0	13.98%	13.98%
13 DMSO	-4.98219306	-4.9817979	99.977844	99.9778292	63.0	36.99%	36.99%
13	-4.98219306	-4.9817979	99.977844	99.9778292	80.0	19.98%	19.98%
14 CDCl3	-2.38536425	-2.3851636	98.2514158	98.2508335	3.0	96.95%	96.95%
14 DMSO	-2.38536425	-2.3851636	98.2514158	98.2508335	0	0%	0%
14	-2.38536425	-2.3851636	98.2514158	98.2508335	8.0	91.86%	91.86%
15 CDCl3	-3.20763014	-3.2078286	99.5581278	99.5582752	85.0	14.62%	14.62%
15 DMSO	-3.20763014	-3.2078286	99.5581278	99.5582752	99.0	0.56%	0.56%
15	-3.20763014	-3.2078286	99.5581278	99.5582752	89.0	10.60%	10.61%
16	N/A	N/A	N/A	N/A	80.0	N/A	N/A
17	-4.6022251	-4.60152716	99.957917	99.95786716	91.7	8.26%	8.26%
18	-6.429058	-6.42883483	99.998076	99.9980748	91.7	8.30%	8.30%
19	-5.8774951	-5.87725398	99.995115	99.99511299	95.8	4.20%	4.20%
20	6.6110987	6.610812583	0.0014151	0.001415785	95.3	6734406.40%	6731148.04%
21	-5.3744423	-5.37524638	99.988576	99.98859132	98.0	1.99%	1.99%
22	-4.0467756	-4.04680877	99.892541	99.89254666	82.1	17.81%	17.81%

23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-6.0214544	-6.02158116	99.996169	99.99617012	93.4	6.60%	6.60%
25	7.195998	7.196278946	0.000527	0.000526702	91.6	17381304.17%	17391138.31%
26	-5.7162902	-5.71598404	99.993586	99.99358307	93.7	6.29%	6.29%
27	-4.5303643	-4.53061859	99.952489	99.9525093	85.2	14.76%	14.76%
28	-4.4686121	-4.46849515	99.947269	99.94725844	88.5	11.45%	11.45%
29	-5.2069258	-5.20770134	99.984841	99.98486047	89.2	10.79%	10.79%
30	-4.1569583	-4.15662293	99.910771	99.91072069	90.8	9.12%	9.12%
31	-5.4745404	-5.47439288	99.990353	99.99035018	93.4	6.59%	6.59%
32	-4.0859302	-4.08634186	99.89941	99.89947994	93.7	6.21%	6.21%
33	-7.0442278	-7.04442165	99.999319	99.99931931	94.6	5.40%	5.40%
34	-4.9901681	-4.99058305	99.97814	99.97815568	93.9	6.08%	6.08%
35	-4.9934444	-4.99309309	99.978261	99.97824807	95.9	4.08%	4.08%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	-4.9308847	-4.93096965	99.975839	99.97584236	97.4	2.58%	2.58%
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	-6.1040559	-6.10441242	99.996668	99.9966701	98.1	1.90%	1.90%
41 $CDCl_3$	-3.68105641	-3.6809707	99.800887	99.80085866	40.5	59.42%	59.42%
42 $CDCl_3$	-5.43124419	-5.4304672	99.989621	99.98960713	92.6	7.39%	7.39%

43 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-7.43342115	-7.4334775	99.9996471	99.9996472	90.2	9.80%	9.80%
44 Acetone	-7.43342115	-7.4334775	99.9996471	99.9996472	93.6	6.40%	6.40%
44 CDCl3	-7.43342115	-7.4334775	99.9996471	99.9996472	91.6	8.40%	8.40%
45 DMSO	-5.78891992	-5.7894026	99.9943267	99.9943314	94.6	5.39%	5.39%
45Acetone	-5.78891992	-5.7894026	99.9943267	99.9943314	99.3	0.69%	0.69%
45 CDCl3	-5.78891992	-5.7894026	99.9943267	99.9943314	97.3	2.69%	2.69%
46 DMSO	N/A	N/A	N/A	N/A	93.7	N/A	N/A
46 Acetone	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 CDCl3	N/A	N/A	N/A	N/A	95.7	N/A	N/A
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	10.21412084	10.2139721	3.221E-6	3.2218E-6	90.7	2815895584.57%	2815196374.02%
48 Acetone	10.21412084	10.2139721	3.221E-6	3.2218E-6	95.3	2958708375.63%	2957973703.46%
48 CDCl3	10.21412084	10.2139721	3.221E-6	3.2218E-6	95.2	2955603749.74%	2954869848.48%
49 DMSO	-5.87609536	-5.8753714	99.9951034	99.9950974	82.5	17.50%	17.50%
49 Acetone	-5.87609536	-5.8753714	99.9951034	99.9950974	92.0	8.00%	8.00%

49 CDCl3	-5.87609536	-5.8753714	99.9951034	99.9950974	88.2	11.80%	11.80%
50 DMSO	10.96470986	10.965101	9.0666E-7	9.0606E-7	94.6	10433900149.27%	10440809559.40%
50 Acetone	10.96470986	10.965101	9.0666E-7	9.0606E-7	97.8	10786843920.91%	10793987053.17%
50 CDCl3	10.96470986	10.965101	9.0666E-7	9.0606E-7	97.2	10720666963.73%	10727766273.09%
51 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	-5.7756307	-5.7755974	99.994198	99.9941976	95.0	4.99%	4.99%
52 Acetone	-5.7756307	-5.7755974	99.994198	99.9941976	96.7	3.29%	3.29%
52 CDCl3	-5.7756307	-5.7755974	99.994198	99.9941976	97.9	2.09%	2.09%
Mean Error of Theoretical Calculation of Gas Phase vs literature						6.78E6%	6.79E6%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.81%	14.81%

Table 1.2: Convergence results from B3LYP-631++G gas phase and how it compares to experimental data.

1.1.3 B3LYP 6-31+G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.455985625	-0.456199406	68.35489508	68.36270472	41.7	38.99%	39.00%
2 ethanol	-47189.98806	-47189.98762	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.0309512	-0.030747965	51.30656595	51.29799055	44.1	14.05%	14.03%
4 ethanol	-0.034258739	-0.034513023	51.44611547	51.45684311	48.3	6.12%	6.13%
5 ethanol	-0.36365342	-0.363328001	64.88952499	64.87700214	47.6	26.64%	26.63%
6	16.78579139	16.78525162	4.87202E-11	4.87647E-11	6E-7	1231422.04%	1230298.22%
7	16.01895359	16.01969003	1.77902E-10	1.77681E-10	1.1E-6	618217.95%	618987.02%
8	15.04462925	15.04454026	9.22238E-10	9.22376E-10	1E-6	108331.88%	108315.66%
9	12.71595146	12.71648002	4.70886E-8	4.70466E-8	4E-5	84846.25%	84922.08%
10	10.60246558	10.60240051	1.67166E-6	1.67184E-6	5.5E-4	32801.43%	32797.88%
11	7.592184344	7.59286495	0.00026988	0.00026957	1.4E-2	5087.49%	5093.46%
12	32.0044958	32.00486703	3.34864E-22	3.34655E-22	0	0%	0%
13 CDCl3	-5.170900764	-10.28130579	99.98388979	99.99999712	86.0	13.99%	14.00%
13 DMSO	-5.170900764	-10.28130579	99.98388979	99.99999712	63.0	36.99%	37.00%
13	-5.170900764	-10.28130579	99.98388979	99.99999712	80.0	19.99%	20%
14 CDCl3	-2.344107993	-2.343747983	98.12759349	98.12647599	3.0	96.94%	96.94%

14 DMSO	-2.344107993	-2.343747983	98.12759349	98.12647599	0	0%	0%
14	-2.344107993	-2.343747983	98.12759349	98.12647599	8.0	91.85%	91.85%
15 CDCl3	-3.188836063	-3.189003279	99.54394188	99.54407008	85.0	14.61%	14.61%
15 DMSO	-3.188836063	-3.189003279	99.54394188	99.54407008	99.0	0.55%	0.55%
15	-3.188836063	-3.189003279	99.54394188	99.54407008	89.0	10.59%	10.59%
16	-3.218052716	-3.21786872	99.56580452	99.56567015	80.0	19.65%	19.65%
17	-4.574756812	-4.57454425	99.95591933	99.95590351	91.7	8.26%	8.26%
18	-6.561030871	-6.56123933	99.99846003	99.99846058	91.7	8.30%	8.30%
19	-5.837674452	-5.83709337	99.99477515	99.99477002	95.8	4.19%	4.19%
20	6.662707234	6.662268362	0.00129698	0.001297942	95.3	7347738.83%	7342292.80%
21	-5.355707369	-5.35516607	99.9882086	99.98819782	98.0	1.99%	1.99%
22	-3.980818077	-3.98092027	99.87989288	99.87991359	82.1	17.80%	17.80%
23	-4.436101115	-4.43586466	99.94429413	99.94427189	91.6	8.35%	8.35%
24	-5.987707671	-5.98706814	99.99594463	99.99594025	93.4	6.60%	6.60%
25	7.252952653	7.252754801	0.000478624	0.000478784	91.6	19138096.16%	19131700.56%
26	-5.644380306	-5.64507546	99.99275823	99.99276672	93.7	6.29%	6.29%
27	-4.569629813	-4.56952418	99.95553614	99.95552821	85.2	14.76%	14.76%
28	-4.391012726	-4.39131148	99.93988901	99.93991931	88.5	11.45%	11.45%
29	-5.181936316	-5.18134594	99.98418723	99.98417146	89.2	10.79%	10.79%
30	N/A	N/A	N/A	N/A	90.8	N/A	N/A

31	-5.428916107	-5.42858468	99.98957987	99.98957404	93.4	6.59%	6.59%
32	-4.029405917	-4.0292385	99.88934503	99.88931378	93.7	6.20%	6.20%
33	-7.034659139	-7.0343815	99.99930799	99.99930767	94.6	5.40%	5.40%
34	-5.035996196	-5.03639125	99.97976817	99.97978166	93.9	6.08%	6.08%
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	-6.116813275	-6.11696261	99.99673912	99.99673994	98.1	1.90%	1.90%
41 CDCl3	-4.391012726	-4.391311481	99.93988901	99.93991931	40.5	59.48%	59.48%
42 CDCl3	-5.181936316	-5.181345942	99.98418723	99.98417146	92.6	7.39%	7.39%
43 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-7.537499405	-7.537016605	99.99673912	99.99673994	90.2	9.80%	9.80%
44 Acetone	-7.537499405	-7.537016605	99.99673912	99.99673994	93.6	6.40%	6.40%
44 CDCl3	-7.537499405	-7.537016605	99.99673912	99.99673994	91.6	8.40%	8.40%
45 DMSO	-6.927048209	-6.92707737	99.7598252	99.75961308	94.6	5.17%	5.17%
45Acetone	-6.927048209	-6.92707737	99.7598252	99.75961308	99.3	0.46%	0.46%

45 CDCl3	-6.927048209	-6.92707737	99.7598252	99.75961308	97.3	2.47%	2.47%
46 DMSO	-6.07862946	-6.078684526	99.98857945	99.98856712	93.7	6.29%	6.29%
46 Acetone	-6.07862946	-6.078684526	99.98857945	99.98856712	97.3	2.69%	2.69%
46 CDCl3	-6.07862946	-6.078684526	99.98857945	99.98856712	95.7	4.29%	4.29%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	-6.247963412	-6.248739601	99.997387	99.99739042	90.7	9.30%	9.30%
48 Acetone	-6.247963412	-6.248739601	99.997387	99.99739042	95.3	4.70%	4.70%
48 CDCl3	-6.247963412	-6.248739601	99.997387	99.99739042	95.2	4.80%	4.80%
49 DMSO	-6.945846953	-6.945902656	99.999196	99.99919608	82.5	17.50%	17.50%
49 Acetone	-6.945846953	-6.945902656	99.999196	99.99919608	92.0	8.00%	8.00%
49 CDCl3	-6.945846953	-6.945902656	99.999196	99.99919608	88.2	11.80%	11.80%
50 DMSO	-6.068880152	-6.068644375	99.99646416	99.99646275	94.6	5.40%	5.40%
50 Acetone	-6.068880152	-6.068644375	99.99646416	99.99646275	97.8	2.20%	2.20%
50 CDCl3	-6.068880152	-6.068644375	99.99646416	99.99646275	97.2	2.80%	2.80%
51 DMSO	-5.696396507	-5.695903731	99.99336724	99.99336172	94.0	5.99%	5.99%
51 Acetone	-5.696396507	-5.695903731	99.99336724	99.99336172	96.4	3.59%	3.59%
51 CDCl3	-5.696396507	-5.695903731	99.99336724	99.99336172	96.1	3.89%	3.89%
52 DMSO	-5.612403862	-5.612444968	99.9923564	99.99235693	95.0	4.99%	4.99%

52 Acetone	-5.612403862	-5.612444968	99.9923564	99.99235693	96.7	3.29%	3.29%
52 CDCl3	-5.612403862	-5.612444968	99.9923564	99.99235693	97.9	2.09%	2.09%
Mean Error of Theoretical Calculation of Gas Phase vs literature						4.39E3%	4.39E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.61%	12.62%

Table 1.3: Convergence results from B3LYP-631+G gas phase and how it compares to experimental data.

1.1.4 B3LYP 6-31G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.6931457	-0.693398	76.32674482	76.33444342	41.7	45.37%	45.37%
2 ethanol	-47188.25008	-47188.25	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.087889892	-0.0884788	53.70420686	53.7289368	44.1	17.88%	17.92%
4 ethanol	-0.246772632	-0.2472387	60.27131303	60.29016172	48.3	19.86%	19.89%
5 ethanol	-0.510549742	-0.5101652	70.3137816	70.30022399	47.6	32.30%	32.29%
6	17.59959156	17.5997589	1.23251E-11	1.23216E-11	6E-7	4868014.66%	4869397.47%
7	17.54840806	17.5489307	1.3438E-11	1.34261E-11	1.1E-6	8185641.93%	8192897.22%
8	15.87372867	15.8734803	2.27354E-10	2.27449E-10	1E-6	439742.71%	439559.00%
9	13.61887588	13.6188387	1.02477E-8	1.02483E-8	4E-5	390231.49%	390208.64%
10	12.06794927	12.0676352	1.40677E-7	1.40751E-7	5.5E-4	390866.54%	390660.99%
11	9.396816678	9.39695476	1.28081E-5	1.28051E-5	1.4E-2	109205.83%	109231.44%
12	33.27553655	33.2762013	3.91352E-23	3.90913E-23	0	0%	0%
13 CDCl3	-5.258208921	-5.2579021	99.98609821	99.986091	86.0	13.99%	13.99%
13 DMSO	-5.258208921	-5.2579021	99.98609821	99.986091	63.0	36.99%	36.99%
13	-5.258208921	-5.2579021	99.98609821	99.986091	80.0	19.99%	19.99%
14 CDCl3	-2.429694308	-2.4297168	98.37550326	98.37556392	3.0	96.95%	96.95%
14 DMSO	-2.429694308	-2.4297168	98.37550326	98.37556392	0	0%	0%

14	-2.429694308	-2.4297168	98.37550326	98.37556392	8.0	91.87%	91.87%
15 CDCl3	-3.563912765	-3.564254	99.75743183	99.75757124	85.0	14.79%	14.79%
15 DMSO	-3.563912765	-3.564254	99.75743183	99.75757124	99.0	0.76%	0.76%
15	-3.563912765	-3.564254	99.75743183	99.75757124	89.0	10.78%	10.78%
16	-3.2627951	-3.262	99.597279	99.6	80.0	19.68%	19.68%
17	-5.5219946	-5.522	99.991096	99.99	91.7	8.29%	8.29%
18	-7.2813287	-7.282	99.999544	100	91.7	8.30%	8.30%
19	-5.8821486	-5.882	99.995153	100	95.8	4.20%	4.20%
20	6.7703965	6.771	0.0010813	0.001	95.3	8813365.27%	9529900%
21	-4.8988599	-4.899	99.974496	99.97	98.0	1.97%	1.97%
22	-4.3297977	-4.33	99.933346	99.93	82.1	17.85%	17.84%
23	-4.5353147	-4.535	99.952884	99.95	91.6	8.36%	8.35%
24	-6.4707877	-6.47	99.998206	100	93.4	6.60%	6.60%
25	7.8047088	7.804	0.0001885	2E-4	91.6	48594064.46%	45799900%
26	-5.8208339	-5.821	99.994624	99.99	93.7	6.29%	6.29%
27	-7.1413251	-7.141	99.999422	100	85.2	14.80%	14.80%
28	-4.2760211	-4.276	99.927013	99.93	88.5	11.44%	11.44%
29	-7.6826048	-7.683	99.999768	100	89.2	10.80%	10.80%
30	-4.0870989	-4.086	99.899608	99.9	90.8	9.11%	9.11%
31	-3.7909622	-3.791	99.834564	99.83	93.4	6.45%	6.44%

32	-4.1072191	-4.107	99.902959	99.9	93.7	6.21%	6.21%
33	-4.4770439	-4.477	99.948014	99.95	94.6	5.35%	5.35%
34	-4.7751521	-4.775	99.968572	99.97	93.9	6.07%	6.07%
35	-4.9352899	-4.936	99.976018	99.98	95.9	4.08%	4.08%
36	-4.8517933	-4.852	99.972387	99.97	95.6	4.37%	4.37%
37	-5.7513358	-5.752	99.993955	99.99	97.0	2.99%	2.99%
38	-4.6150508	-4.615	99.958818	99.96	97.4	2.56%	2.56%
39	-5.333103	-5.333	99.98775	99.99	96.8	3.19%	3.19%
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-3.995698975	-3.995353	99.88287041	99.88280203	40.5	59.45%	59.45%
42 CDCl3	-6.03497207	-6.0353864	99.99625576	99.99625838	92.6	7.40%	7.40%
43 DMSO	-5.875119849	-5.8753714	99.99509534	99.99509742	94.0	6.00%	6.00%
43 Acetone	-5.875119849	-5.8753714	99.99509534	99.99509742	97.7	2.30%	2.30%
43 CDCl3	-5.875119849	-5.8753714	99.99509534	99.99509742	97.8	2.20%	2.20%
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-6.517648409	-6.5173137	99.99834297	99.99834203	94.6	5.40%	5.40%
45Acetone	-6.517648409	-6.5173137	99.99834297	99.99834203	99.3	0.70%	0.70%
45 CDCl3	-6.517648409	-6.5173137	99.99834297	99.99834203	97.3	2.70%	2.70%

46 DMSO	-5.804781004	-5.8044629	99.99447669	99.99447372	93.7	6.29%	6.29%
46 Acetone	-5.804781004	-5.8044629	99.99447669	99.99447372	97.3	2.69%	2.69%
46 CDCl3	-5.804781004	-5.8044629	99.99447669	99.99447372	95.7	4.29%	4.29%
47 DMSO	-6.728332296	-6.7281569	99.99883909	99.99883875	70.1	29.90%	29.90%
47 Acetone	-6.728332296	-6.7281569	99.99883909	99.99883875	87.1	12.90%	12.90%
47 CDCl3	-6.728332296	-6.7281569	99.99883909	99.99883875	86.6	13.40%	13.40%
48 DMSO	-4.488833785	-4.4885755	99.94903848	99.94901625	90.7	9.25%	9.25%
48 Acetone	-4.488833785	-4.4885755	99.94903848	99.94901625	95.3	4.65%	4.65%
48 CDCl3	-4.488833785	-4.4885755	99.94903848	99.94901625	95.2	4.75%	4.75%
49 DMSO	-6.78225755	-6.7821227	99.99894015	99.99893991	82.5	17.50%	17.50%
49 Acetone	-6.78225755	-6.7821227	99.99894015	99.99893991	92.0	8.00%	8.00%
49 CDCl3	-6.78225755	-6.7821227	99.99894015	99.99893991	88.2	11.80%	11.80%
50 DMSO	-5.68691082	-5.6864911	99.99326013	99.99325535	94.6	5.39%	5.39%
50 Acetone	-5.68691082	-5.6864911	99.99326013	99.99325535	97.8	2.19%	2.19%
50 CDCl3	-5.68691082	-5.6864911	99.99326013	99.99325535	97.2	2.79%	2.79%
51 DMSO	-5.700133006	-5.6996688	99.99340897	99.9934038	94.0	5.99%	5.99%
51 Acetone	-5.700133006	-5.6996688	99.99340897	99.9934038	96.4	3.59%	3.59%
51 CDCl3	-5.700133006	-5.6996688	99.99340897	99.9934038	96.1	3.89%	3.89%
52 DMSO	-5.766280472	-5.7655573	99.99410563	99.99409842	95.0	4.99%	4.99%
52 Acetone	-5.766280472	-5.7655573	99.99410563	99.99409842	96.7	3.29%	3.29%

52 CDCl3	-5.766280472	-5.7655573	99.99410563	99.99409842	97.9	2.09%	2.09%
Mean Error of Theoretical Calculation of Gas Phase vs literature						9.83E3%	9.55E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.56%	12.56%

Table 1.4: Convergence results from B3LYP-631G gas phase and how it compares to experimental data.

1.1.5 B3LYP cc-pVDZ

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	N/A	N/A	N/A	N/A	41.7	N/A	N/A
2 ethanol	-47192.7	-47192.7	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.12002	-0.12048	55.05027	55.06967	44.1	19.89%	19.92%
4 ethanol	0.453862	0.453689	31.72274	31.72905	48.3	52.26%	52.23%
5 ethanol	-0.26769	-0.26795	61.11422	61.12439	47.6	22.11%	22.13%
6	16.70366	16.70368	5.6E-11	5.6E-11	6.00E-7	1071907.78%	1071937.95%
7	16.58395	16.58382	6.85E-11	6.85E-11	1.10E-6	1605491.33%	1605136.69%
8	14.98903	14.98932	1.01E-9	1.01E-9	1.00E-6	98612.68%	98661.51%
9	12.8852	12.88528	3.54E-8	3.54E-8	4.00E-5	112953.62%	112969.59%
10	11.31701	11.31713	5E-7	5E-7	5.50E-4	109884.46%	109907.28%
11	9.038229	9.038019	2.35E-5	2.35E-5	1.40E-2	59551.61%	59530.47%
12	31.89097	31.89129	4.06E-22	4.05E-22	0	0%	0%
13 CDCl3	-5.58919	-5.5886	99.99205	99.99204	86	13.99%	13.99%
13 DMSO	-5.58919	-5.5886	99.99205	99.99204	63	36.99%	36.99%
13	-5.58919	-5.5886	99.99205	99.99204	80	19.99%	19.99%
14 CDCl3	-3.10485	-3.10492	99.47481	99.47486	3	96.98%	96.98%
14 DMSO	-3.10485	-3.10492	99.47481	99.47486	0	0%	0%

14	-3.10485	-3.10492	99.47481	99.47486	8	91.96%	91.96%
15 CDCl3	-4.18938	-4.18925	99.91552	99.9155	85	14.93%	14.93%
15 DMSO	-4.18938	-4.18925	99.91552	99.9155	99	0.92%	0.92%
15	-4.18938	-4.18925	99.91552	99.9155	89	10.92%	10.92%
16	-3.58039	-3.57994	99.76407	99.7639	80	19.81%	19.81%
17	-5.62728	-5.62688	99.99255	99.99254	91.7	8.29%	8.29%
18	-7.69538	-7.69515	99.99977	99.99977	91.7	8.30%	8.30%
19	-6.73769	-6.73757	99.99886	99.99886	95.8	4.20%	4.20%
20	N/A	N/A	N/A	N/A	95.3	N/A	N/A
21	-5.41286	-5.4129	99.98929	99.98929	98	1.99%	1.99%
22	-4.76133	-4.76154	99.96783	99.96784	82.1	17.87%	17.87%
23	-4.94518	-4.94603	99.97642	99.97645	91.6	8.38%	8.38%
24	-7.17225	-7.17181	99.99945	99.99945	93.4	6.60%	6.60%
25	7.273805	7.27409	0.000462	0.000462	91.6	19824080.47%	19833644.11%
26	-6.49652	-6.49598	99.99828	99.99828	93.7	6.30%	6.30%
27	-7.74873	-7.74849	99.99979	99.99979	85.2	14.80%	14.80%
28	-4.72339	-4.72326	99.9657	99.96569	88.5	11.47%	11.47%
29	-8.26122	-8.26116	99.99991	99.99991	89.2	10.80%	10.80%
30	-7.10722	-7.10717	99.99939	99.99939	90.8	9.20%	9.20%
31	-6.16883	-6.16905	99.99701	99.99701	93.4	6.60%	6.60%

32	-4.68237	-4.68248	99.96324	99.96325	93.7	6.27%	6.27%
33	-4.95936	-4.95921	99.97697	99.97697	94.6	5.38%	5.38%
34	-5.53842	-5.53777	99.99134	99.99133	93.9	6.09%	6.09%
35	-5.6414	-5.64194	99.99272	99.99273	95.9	4.09%	4.09%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	-6.58164	-6.58195	99.99851	99.99851	97	3.00%	3.00%
38	-5.60458	-5.60429	99.99225	99.99225	97.4	2.59%	2.59%
39	-6.0952	-6.095	99.99662	99.99662	96.8	3.20%	3.20%
40	-7.67608	-7.67632	99.99977	99.99977	98.1	1.90%	1.90%
41 CDCl3	-4.16908	-4.16917	99.91258	99.91259	40.5	59.46%	59.46%
42 CDCl3	-6.60603	-6.60642	99.99857	99.99857	92.6	7.40%	7.40%
43 DMSO	-7.38781	-7.38767	99.99962	99.99962	94	6.00%	6.00%
43 Acetone	-7.38781	-7.38767	99.99962	99.99962	97.7	2.30%	2.30%
43 CDCl3	-7.38781	-7.38767	99.99962	99.99962	97.8	2.20%	2.20%
44 DMSO	-7.40066	-7.40022	99.99963	99.99963	90.2	9.80%	9.80%
44 Acetone	-7.40066	-7.40022	99.99963	99.99963	93.6	6.40%	6.40%
44 CDCl3	-7.40066	-7.40022	99.99963	99.99963	91.6	8.40%	8.40%
45 DMSO	-6.43998	-6.44013	99.99811	99.99811	94.6	5.40%	5.40%
45Acetone	-6.43998	-6.44013	99.99811	99.99811	99.3	0.70%	0.70%
45 CDCl3	-6.43998	-6.44013	99.99811	99.99811	97.3	2.70%	2.70%

46 DMSO	-8.42943	-8.42934	99.99993	99.99993	93.7	6.30%	6.30%
46 Acetone	-8.42943	-8.42934	99.99993	99.99993	97.3	2.70%	2.70%
46 CDCl3	-8.42943	-8.42934	99.99993	99.99993	95.7	4.30%	4.30%
47 DMSO	-7.4742	-7.47364	99.99967	99.99967	70.1	29.90%	29.90%
47 Acetone	-7.4742	-7.47364	99.99967	99.99967	87.1	12.90%	12.90%
47 CDCl3	-7.4742	-7.47364	99.99967	99.99967	86.6	13.40%	13.40%
48 DMSO	-7.31511	-7.31488	99.99957	99.99957	90.7	9.30%	9.30%
48 Acetone	-7.31511	-7.31488	99.99957	99.99957	95.3	4.70%	4.70%
48 CDCl3	-7.31511	-7.31488	99.99957	99.99957	95.2	4.80%	4.80%
49 DMSO	-7.01631	-7.01681	99.99929	99.99929	82.5	17.50%	17.50%
49 Acetone	-7.01631	-7.01681	99.99929	99.99929	92	8.00%	8.00%
49 CDCl3	-7.01631	-7.01681	99.99929	99.99929	88.2	11.80%	11.80%
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	-7.03915	-7.03877	99.99931	99.99931	94	6.00%	6.00%
51 Acetone	-7.03915	-7.03877	99.99931	99.99931	96.4	3.60%	3.60%
51 CDCl3	-7.03915	-7.03877	99.99931	99.99931	96.1	3.90%	3.90%
52 DMSO	-6.82668	-6.8273	99.99902	99.99902	95	5.00%	5.00%
52 Acetone	-6.82668	-6.8273	99.99902	99.99902	96.7	3.30%	3.30%

52 CDCl3	-6.82668	-6.8273	99.99902	99.99902	97.9	2.10%	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						3.22E3%	3.22E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.63%	12.63%

Table 1.5: Convergence results from B3LYP cc-pVDZ gas phase and how it compares to experimental data.

1.2 CAM-B3LYP gas phase

1.2.1 CAM-B3LYP 6-311++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-1.13293	-1.13265	87.14065	87.13535	41.7	52.15%	52.14%
2 ethanol	-47191	-47191	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.79506	-0.79568	79.29506	79.31231	44.1	44.38%	44.40%
4 ethanol	-0.61692	-0.61621	73.92233	73.89938	48.3	34.66%	34.64%
5 ethanol	-0.99026	-0.99021	84.19058	84.18955	47.6	43.46%	43.46%
6	15.40139	15.40159	5.05E-10	5.05E-10	6.00E-7	118748.17%	118788.44%
7	15.49406	15.49446	4.32E-10	4.31E-10	1.10E-6	254701.92%	254877.44%
8	14.70216	14.70255	1.64E-9	1.64E-9	1.00E-6	60707.78%	60747.41%
9	12.31719	12.31738	9.23E-8	9.23E-8	4.00E-5	43216.50%	43230.83%
10	10.15035	10.15059	3.59E-6	3.59E-6	5.50E-4	15231.76%	15238.06%
11	7.371549	7.371354	0.000392	0.000392	1.40E-2	3473.74%	3472.56%
12	31.58485	31.58506	6.8E-22	6.8E-22	0	0	0
13 CDCl3	-4.10435	-4.10391	99.90249	99.90242	86	13.92%	13.92%
13 DMSO	-4.10435	-4.10391	99.90249	99.90242	63	36.94%	36.94%
13	-4.10435	-4.10391	99.90249	99.90242	80	19.92%	19.92%
14 CDCl3	-1.33764	-1.33722	90.54403	90.53796	3	96.69%	96.69%

14 DMSO	-1.33764	-1.33722	90.54403	90.53796	0	0	0
14	-1.33764	-1.33722	90.54403	90.53796	8	91.16%	91.16%
15 CDCl3	-2.62005	-2.61985	98.81685	98.81646	85	13.98%	13.98%
15 DMSO	-2.62005	-2.61985	98.81685	98.81646	99	0.19%	0.19%
15	-2.62005	-2.61985	98.81685	98.81646	89	9.93%	9.93%
16	-2.26186	-2.26217	97.85457	97.85565	80	18.25%	18.25%
17	-3.77796	-3.77761	99.8309	99.8308	91.7	8.14%	8.14%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-5.11583	-5.11546	99.98232	99.98231	95.8	4.18%	4.18%
20	7.045807	7.045677	0.000679	0.000679	95.3	14033170.89%	14030071.99%
21	-3.9416	-3.94139	99.87168	99.87163	98	1.87%	1.87%
22	-3.19718	-3.19716	99.5503	99.55028	82.1	17.53%	17.53%
23	-3.48582	-3.48519	99.72333	99.72303	91.6	8.15%	8.15%
24	-5.07857	-5.07906	99.98117	99.98119	93.4	6.58%	6.58%
25	7.709479	7.709582	0.000221	0.000221	91.6	41376896.55%	41384091.68%
26	-4.88715	-4.88767	99.97399	99.97401	93.7	6.28%	6.28%
27	-3.64538	-3.6452	99.78855	99.78848	85.2	14.62%	14.62%
28	-3.34024	-3.34023	99.64648	99.64648	88.5	11.19%	11.19%
29	-4.08191	-4.08195	99.89873	99.89873	89.2	10.71%	10.71%
30	-5.89669	-5.89671	99.99527	99.99527	90.8	9.20%	9.20%

31	-4.47447	-4.47414	99.94779	99.94776	93.4	6.55%	6.55%
32	-2.99554	-2.99573	99.36899	99.36919	93.7	5.70%	5.71%
33	-5.96769	-5.96762	99.99581	99.9958	94.6	5.40%	5.40%
34	-3.38297	-3.38228	99.67101	99.67063	93.9	5.79%	5.79%
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	-4.54985	-4.54944	99.95403	99.95399	97	2.96%	2.96%
38	-3.68571	-3.68599	99.80244	99.80254	97.4	2.41%	2.41%
39	-3.78792	-3.78765	99.83371	99.83364	96.8	3.04%	3.04%
40	-4.88714	-4.88704	99.97399	99.97398	98.1	1.87%	1.87%
41 CDCl3	-2.51202	-2.51192	98.5834	98.58316	40.5	58.92%	58.92%
42 CDCl3	-4.348	-4.34801	99.93536	99.93536	92.6	7.34%	7.34%
43 DMSO	-4.49467	-4.49422	99.94954	99.9495	94	5.95%	5.95%
43 Acetone	-4.49467	-4.49422	99.94954	99.9495	97.7	2.25%	2.25%
43 CDCl3	-4.49467	-4.49422	99.94954	99.9495	97.8	2.15%	2.15%
44 DMSO	-5.91501	-5.9149	99.99541	99.99541	90.2	9.80%	9.80%
44 Acetone	-5.91501	-5.9149	99.99541	99.99541	93.6	6.40%	6.40%
44 CDCl3	-5.91501	-5.9149	99.99541	99.99541	91.6	8.40%	8.40%
45 DMSO	-5.14751	-5.14809	99.98324	99.98326	94.6	5.38%	5.38%
45Acetone	-5.14751	-5.14809	99.98324	99.98326	99.3	0.68%	0.68%

45 CDCl3	-5.14751	-5.14809	99.98324	99.98326	97.3	2.68%	2.68%
46 DMSO	-4.51602	-4.51619	99.95132	99.95134	93.7	6.25%	6.25%
46 Acetone	-4.51602	-4.51619	99.95132	99.95134	97.3	2.65%	2.65%
46 CDCl3	-4.51602	-4.51619	99.95132	99.95134	95.7	4.25%	4.25%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95	N/A	N/A

52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						9.98E3%	9.98E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						15.23%	15.23%

Table 1.6: Convergence results from CAM-B3LYP-6-311++G gas phase and how it compares to experimental data.

1.2.2 CAM-B3LYP 6-31++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-1.17067	-1.17093	87.8381	87.84281	41.7	52.53%	52.53%
2 ethanol	-47178.4	-47178.4	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.9506	-0.95068	83.27869	83.28039	44.1	47.05%	47.05%
4 ethanol	-0.72184	-0.72226	77.19124	77.20381	48.3	37.43%	37.44%
5 ethanol	-1.16309	-1.16278	87.70058	87.69491	47.6	45.72%	45.72%
6	16.26093	16.26128	1.18E-10	1.18E-10	6.00E-7	507428.66%	507727.62%
7	16.05715	16.05671	1.67E-10	1.67E-10	1.10E-6	659419.46%	658934.45%
8	15.28137	15.28111	6.18E-10	6.19E-10	1.00E-6	161635.58%	161564.85%
9	12.81564	12.81625	3.98E-8	3.98E-8	4.00E-5	100422.12%	100527.24%
10	10.70373	10.70406	1.41E-6	1.41E-6	5.50E-4	38938.50%	38960.05%
11	7.639436	7.639928	0.000249	0.000249	1.40E-2	5518.44%	5523.11%
12	32.03962	32.03938	3.16E-22	3.16E-22	0	0%	0%
13 CDCl3	-4.74193	-4.74272	99.96676	99.9668	86	13.97%	13.97%
13 DMSO	-4.74193	-4.74272	99.96676	99.9668	63	36.98%	36.98%
13	-4.74193	-4.74272	99.96676	99.9668	80	19.97%	19.97%
14 CDCl3	-1.7348	-1.73444	94.93077	94.92783	3	96.84%	96.84%
14 DMSO	-1.7348	-1.73444	94.93077	94.92783	0	0%	0%

14	-1.7348	-1.73444	94.93077	94.92783	8	91.57%	91.57%
15 CDCl3	-3.1789	-3.17896	99.53626	99.53631	85	14.60%	14.60%
15 DMSO	-3.1789	-3.17896	99.53626	99.53631	99	0.54%	0.54%
15	-3.1789	-3.17896	99.53626	99.53631	89	10.59%	10.59%
16	-2.95737	-2.95808	99.32725	99.32805	80	19.46%	19.46%
17	-4.67066	-4.67055	99.96251	99.9625	91.7	8.27%	8.27%
18	-6.4829	-6.4828	99.99824	99.99824	91.7	8.30%	8.30%
19	-5.74382	-5.74422	99.99388	99.99388	95.8	4.19%	4.19%
20	6.975637	6.974768	0.000765	0.000766	95.3	12464815.41%	12446544.94%
21	-4.95518	-4.95544	99.97681	99.97682	98	1.98%	1.98%
22	-3.84414	-3.84412	99.84875	99.84875	82.1	17.78%	17.78%
23	-4.30551	-4.30534	99.93056	99.93054	91.6	8.34%	8.34%
24	-5.76789	-5.76807	99.99412	99.99412	93.4	6.59%	6.59%
25	7.768099	7.76794	0.000201	0.000201	91.6	45683081.30%	45670840.71%
26	-5.5747	-5.57542	99.99185	99.99186	93.7	6.29%	6.29%
27	-4.37449	-4.37374	99.93819	99.93811	85.2	14.75%	14.75%
28	-4.05196	-4.05246	99.89348	99.89357	88.5	11.41%	11.41%
29	-4.95917	-4.95921	99.97697	99.97697	89.2	10.78%	10.78%
30	-3.92658	-3.9257	99.86839	99.86819	90.8	9.08%	9.08%
31	-5.21055	-5.21084	99.98493	99.98494	93.4	6.59%	6.59%

32	-3.75448	-3.75439	99.82407	99.82404	93.7	6.13%	6.13%
33	-6.62723	-6.62776	99.99862	99.99862	94.6	5.40%	5.40%
34	-4.19028	-4.19051	99.91565	99.91568	93.9	6.02%	6.02%
35	-4.32753	-4.32731	99.93309	99.93307	95.9	4.04%	4.04%
36	-4.32304	-4.32291	99.93258	99.93257	95.6	4.34%	4.34%
37	-4.9499	-4.94979	99.9766	99.9766	97	2.98%	2.98%
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	-4.63165	-4.63165	99.95996	99.95996	96.8	3.16%	3.16%
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-3.34085	-3.34086	99.64685	99.64685	40.5	59.36%	59.36%
42 CDCl3	-5.39507	-5.39533	99.98897	99.98897	92.6	7.39%	7.39%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-7.23736	-7.23769	99.99951	99.99951	90.2	9.80%	9.80%
44 Acetone	-7.23736	-7.23769	99.99951	99.99951	93.6	6.40%	6.40%
44 CDCl3	-7.23736	-7.23769	99.99951	99.99951	91.6	8.40%	8.40%
45 DMSO	-5.93511	-5.93498	99.99557	99.99557	94.6	5.40%	5.40%
45Acetone	-5.93511	-5.93498	99.99557	99.99557	99.3	0.70%	0.70%
45 CDCl3	-5.93511	-5.93498	99.99557	99.99557	97.3	2.70%	2.70%

46 DMSO	-5.21933	-5.219	99.98515	99.98515	93.7	6.29%	6.29%
46 Acetone	-5.21933	-5.219	99.98515	99.98515	97.3	2.69%	2.69%
46 CDCl3	-5.21933	-5.219	99.98515	99.98515	95.7	4.29%	4.29%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	11.11232	11.11194	7.07E-7	7.07E-7	90.7	12836204869.44%	12827916089.36%
48 Acetone	11.11232	11.11194	7.07E-7	7.07E-7	95.3	13487214162.27%	13478505003.05%
48 CDCl3	11.11232	11.11194	7.07E-7	7.07E-7	95.2	13473061786.34%	13464361765.79%
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-5.01303	-5.01317	99.97897	99.97897	94.6	5.38%	5.38%
50 Acetone	-5.01303	-5.01317	99.97897	99.97897	97.8	2.18%	2.18%
50 CDCl3	-5.01303	-5.01317	99.97897	99.97897	97.2	2.78%	2.78%
51 DMSO	-4.99741	-4.99749	99.97841	99.97841	94	5.98%	5.98%
51 Acetone	-4.99741	-4.99749	99.97841	99.97841	96.4	3.58%	3.58%
51 CDCl3	-4.99741	-4.99749	99.97841	99.97841	96.1	3.88%	3.88%
52 DMSO	N/A	N/A	N/A	N/A	95	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A

52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						6.33E6%	6.32E6%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.82%	14.82%

Table 1.7: Convergence results from CAM-B3LYP-6-31++G gas phase and how it compares to experimental data.

1.2.3 CAM-B3LYP 6-31+G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-1.19395	-1.19415	88.25187	88.2554	41.7	52.75%	52.75%
2 ethanol	-47178.1	-47178.1	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.71323	-0.71348	76.93414	76.94162	44.1	42.68%	42.68%
4 ethanol	-0.68071	-0.68085	75.94514	75.9494	48.3	36.40%	36.41%
5 ethanol	-1.05728	-1.05673	85.63966	85.62813	47.6	44.42%	44.41%
6	16.50592	16.50601	7.82E-11	7.81E-11	6.00E-7	767539.41%	767656.58%
7	16.10003	16.10001	1.55E-10	1.55E-10	1.10E-6	708961.86%	708934.05%
8	15.38421	15.38465	5.2E-10	5.19E-10	1.00E-6	192313.10%	192457.73%
9	12.90152	12.90097	3.44E-8	3.45E-8	4.00E-5	116114.65%	116005.47%
10	10.7873	10.78752	1.22E-6	1.22E-6	5.50E-4	44856.10%	44872.74%
11	7.605267	7.605415	0.000264	0.000264	1.40E-2	5203.38%	5204.71%
12	32.13507	32.13602	2.69E-22	2.68E-22	0	0%	0%
13 CDCl3	-4.86123	-4.86132	99.97282	99.97283	86	13.98%	13.98%
13 DMSO	-4.86123	-4.86132	99.97282	99.97283	63	36.98%	36.98%
13	-4.86123	-4.86132	99.97282	99.97283	80	19.98%	19.98%
14 CDCl3	-1.71871	-1.71812	94.79839	94.7935	3	96.84%	96.84%
14 DMSO	-1.71871	-1.71812	94.79839	94.7935	0	0%	0%

14	-1.71871	-1.71812	94.79839	94.7935	8	91.56%	91.56%
15 CDCl3	-3.1827	-3.18273	99.53921	99.53923	85	14.61%	14.61%
15 DMSO	-3.1827	-3.18273	99.53921	99.53923	99	0.54%	0.54%
15	-3.1827	-3.18273	99.53921	99.53923	89	10.59%	10.59%
16	N/A	N/A	N/A	N/A	80	N/A	N/A
17	-5.24698	-5.24661	99.98583	99.98582	91.7	8.29%	8.29%
18	-6.82085	-6.82103	99.99901	99.99901	91.7	8.30%	8.30%
19	-5.72161	-5.72226	99.99364	99.99365	95.8	4.19%	4.19%
20	7.007033	7.006771	0.000725	0.000725	95.3	13143626.06%	13137805.94%
21	-4.93472	-4.93536	99.976	99.97602	98	1.98%	1.98%
22	-3.80068	-3.80083	99.83725	99.83729	82.1	17.77%	17.77%
23	-4.27301	-4.27334	99.92664	99.92668	91.6	8.33%	8.33%
24	-5.74048	-5.73983	99.99384	99.99384	93.4	6.59%	6.59%
25	7.822276	7.821906	0.000183	0.000183	91.6	50060411.61%	50029096.40%
26	-5.51978	-5.5202	99.99106	99.99107	93.7	6.29%	6.29%
27	-4.35324	-4.35303	99.93593	99.93591	85.2	14.75%	14.75%
28	-3.98144	-3.98155	99.88002	99.88004	88.5	11.39%	11.39%
29	-4.9306	-4.93097	99.97583	99.97584	89.2	10.78%	10.78%
30	-3.87377	-3.87362	99.85613	99.85609	90.8	9.07%	9.07%
31	-5.16775	-5.16817	99.9838	99.98382	93.4	6.58%	6.58%

32	-5.37718	-5.37776	99.98863	99.98864	93.7	6.29%	6.29%
33	-6.59737	-6.59763	99.99855	99.99855	94.6	5.40%	5.40%
34	-4.24102	-4.24071	99.92257	99.92253	93.9	6.03%	6.03%
35	-4.35854	-4.35805	99.9365	99.93645	95.9	4.04%	4.04%
36	-4.3615	-4.36119	99.93682	99.93679	95.6	4.34%	4.34%
37	-5.02305	-5.02321	99.97932	99.97933	97	2.98%	2.98%
38	-4.65411	-4.65487	99.96145	99.9615	97.4	2.56%	2.56%
39	-4.75998	-4.76029	99.96776	99.96777	96.8	3.17%	3.17%
40	-5.66881	-5.66892	99.99305	99.99305	98.1	1.89%	1.89%
41 CDCl3	-3.20766	-3.2072	99.55815	99.55781	40.5	59.32%	59.32%
42 CDCl3	-5.36132	-5.36144	99.98832	99.98832	92.6	7.39%	7.39%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-7.45656	-7.4567	99.99966	99.99966	90.2	9.80%	9.80%
44 Acetone	-7.45656	-7.4567	99.99966	99.99966	93.6	6.40%	6.40%
44 CDCl3	-7.45656	-7.4567	99.99966	99.99966	91.6	8.40%	8.40%
45 DMSO	-6.04059	-6.04041	99.99629	99.99629	94.6	5.40%	5.40%
45Acetone	-6.04059	-6.04041	99.99629	99.99629	99.3	0.70%	0.70%
45 CDCl3	-6.04059	-6.04041	99.99629	99.99629	97.3	2.70%	2.70%

46 DMSO	-5.32939	-5.32881	99.98767	99.98766	93.7	6.29%	6.29%
46 Acetone	-5.32939	-5.32881	99.98767	99.98766	97.3	2.69%	2.69%
46 CDCl3	-5.32939	-5.32881	99.98767	99.98766	95.7	4.29%	4.29%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	-5.43872	-5.43862	99.98975	99.98975	90.7	9.29%	9.29%
48 Acetone	-5.43872	-5.43862	99.98975	99.98975	95.3	4.69%	4.69%
48 CDCl3	-5.43872	-5.43862	99.98975	99.98975	95.2	4.79%	4.79%
49 DMSO	-6.46103	-6.46021	99.99818	99.99817	82.5	17.50%	17.50%
49 Acetone	-6.46103	-6.46021	99.99818	99.99817	92	8.00%	8.00%
49 CDCl3	-6.46103	-6.46021	99.99818	99.99817	88.2	11.80%	11.80%
50 DMSO	-5.30131	-5.30057	99.98707	99.98706	94.6	5.39%	5.39%
50 Acetone	-5.30131	-5.30057	99.98707	99.98706	97.8	2.19%	2.19%
50 CDCl3	-5.30131	-5.30057	99.98707	99.98706	97.2	2.79%	2.79%
51 DMSO	-5.24092	-5.24159	99.98569	99.9857	94	5.99%	5.99%
51 Acetone	-5.24092	-5.24159	99.98569	99.9857	96.4	3.59%	3.59%
51 CDCl3	-5.24092	-5.24159	99.98569	99.9857	96.1	3.89%	3.89%
52 DMSO	-5.08489	-5.08534	99.98137	99.98139	95	4.98%	4.98%
52 Acetone	-5.08489	-5.08534	99.98137	99.98139	96.7	3.28%	3.28%

52 CDCl3	-5.08489	-5.08534	99.98137	99.98139	97.9	2.08%	2.08%
Mean Error of Theoretical Calculation of Gas Phase vs literature						9.29E3%	9.29E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						13.16%	13.16%

Table 1.8: Convergence results from CAM-B3LYP-631+G gas phase and how it compares to experimental data.

1.2.4 CAM-B3LYP 6-31G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	N/A	-1.39182	N/A	91.29887	41.7	N/A	54.33%
2 ethanol	-47192.7	-47176.1	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.12002	-1.08622	55.05027	86.23031	44.1	19.89%	48.86%
4 ethanol	0.453862	-0.86847	31.72274	81.25696	48.3	52.26%	40.56%
5 ethanol	-0.26769	-1.18474	61.11422	88.08962	47.6	22.11%	45.96%
6	16.70366	17.64117	5.6E-11	1.15E-11	6.00E-7	1071907.78%	5222189.39%
7	16.58395	17.58031	6.85E-11	1.27E-11	1.10E-6	1605491.33%	8638745.34%
8	14.98903	16.14519	1.01E-9	1.44E-10	1.00E-6	98612.68%	695587.50%
9	12.8852	13.68724	3.54E-8	9.13E-9	4.00E-5	112953.62%	438003.99%
10	11.31701	12.1718	5E-7	1.18E-7	5.50E-4	109884.46%	465824.88%
11	9.038229	9.282121	2.35E-5	1.55E-5	1.40E-2	59551.61%	89956.52%
12	31.89097	33.33581	4.06E-22	3.53E-23	0	0%	0%
13 CDCl3	-5.58919	-6.30208	99.99205	99.99762	86	13.99%	14.00%
13 DMSO	-5.58919	-6.30208	99.99205	99.99762	63	36.99%	37.00%
13	-5.58919	-6.30208	99.99205	99.99762	80	19.99%	20.00%
14 CDCl3	-3.10485	-2.07392	99.47481	97.07648	3	96.98%	96.91%
14 DMSO	-3.10485	-2.07392	99.47481	97.07648	0	0%	0%

14	-3.10485	-2.07392	99.47481	97.07648	8	91.96%	91.76%
15 CDCl3	-4.18938	-3.60818	99.91552	99.77487	85	14.93%	14.81%
15 DMSO	-4.18938	-3.60818	99.91552	99.77487	99	0.92%	0.78%
15	-4.18938	-3.60818	99.91552	99.77487	89	10.92%	10.80%
16	-3.58039	-3.14947	99.76407	99.51274	80	19.81%	19.61%
17	-5.62728	-5.32818	99.99255	99.98765	91.7	8.29%	8.29%
18	-7.69538	-7.07329	99.99977	99.99935	91.7	8.30%	8.30%
19	-6.73769	-5.97766	99.99886	99.99588	95.8	4.20%	4.20%
20	N/A	6.90637	N/A	0.000859	95.3	N/A	11088653.73%
21	-5.41286	-4.74585	99.98929	99.96698	98	1.99%	1.97%
22	-4.76133	-4.3204	99.96783	99.93228	82.1	17.87%	17.84%
23	-4.94518	-4.34864	99.97642	99.93543	91.6	8.38%	8.34%
24	-7.17225	-6.47715	99.99945	99.99823	93.4	6.60%	6.60%
25	7.273805	8.240455	0.000462	9.03E-5	91.6	19824080.47%	101443935.17%
26	-6.49652	-5.72414	99.99828	99.99367	93.7	6.30%	6.29%
27	-7.74873	-7.11282	99.99979	99.99939	85.2	14.80%	14.80%
28	-4.72339	-4.01292	99.9657	99.88622	88.5	11.47%	11.40%
29	-8.26122	-7.33935	99.99991	99.99959	89.2	10.80%	10.80%
30	-7.10722	-6.31902	99.99939	99.99768	90.8	9.20%	9.20%
31	-6.16883	-3.52598	99.99701	99.74142	93.4	6.60%	6.36%

32	-4.68237	-6.08057	99.96324	99.99653	93.7	6.27%	6.30%
33	-4.95936	-4.19741	99.97697	99.91666	94.6	5.38%	5.32%
34	-5.53842	-4.14094	99.99134	99.90833	93.9	6.09%	6.01%
35	-5.6414	-4.21435	99.99272	99.91901	95.9	4.09%	4.02%
36	N/A	-4.13654	N/A	99.90764	95.6	N/A	4.31%
37	-6.58164	-5.1939	99.99851	99.9845	97	3.00%	2.98%
38	-5.60458	-4.12713	99.99225	99.90617	97.4	2.59%	2.51%
39	-6.0952	-4.26204	99.99662	99.92527	96.8	3.20%	3.13%
40	-7.67608	-5.50702	99.99977	99.99087	98.1	1.90%	1.89%
41 CDCl3	-4.16908	-3.69289	99.91258	99.80482	40.5	59.46%	59.42%
42 CDCl3	-6.60603	-6.13014	99.99857	99.99681	92.6	7.40%	7.40%
43 DMSO	-7.38781	-5.23845	99.99962	99.98563	94	6.00%	5.99%
43 Acetone	-7.38781	-5.23845	99.99962	99.98563	97.7	2.30%	2.29%
43 CDCl3	-7.38781	-5.23845	99.99962	99.98563	97.8	2.20%	2.19%
44 DMSO	-7.40066	-6.46335	99.99963	99.99818	90.2	9.80%	9.80%
44 Acetone	-7.40066	-6.46335	99.99963	99.99818	93.6	6.40%	6.40%
44 CDCl3	-7.40066	-6.46335	99.99963	99.99818	91.6	8.40%	8.40%
45 DMSO	-6.43998	-4.48418	99.99811	99.94864	94.6	5.40%	5.35%
45Acetone	-6.43998	-4.48418	99.99811	99.94864	99.3	0.70%	0.65%
45 CDCl3	-6.43998	-4.48418	99.99811	99.94864	97.3	2.70%	2.65%

46 DMSO	-8.42943	-5.12299	99.99993	99.98253	93.7	6.30%	6.28%
46 Acetone	-8.42943	-5.12299	99.99993	99.98253	97.3	2.70%	2.68%
46 CDCl3	-8.42943	-5.12299	99.99993	99.98253	95.7	4.30%	4.28%
47 DMSO	-7.4742	-6.74886	99.99967	99.99888	70.1	29.90%	29.90%
47 Acetone	-7.4742	-6.74886	99.99967	99.99888	87.1	12.90%	12.90%
47 CDCl3	-7.4742	-6.74886	99.99967	99.99888	86.6	13.40%	13.40%
48 DMSO	-7.31511	-5.62688	99.99957	99.99254	90.7	9.30%	9.29%
48 Acetone	-7.31511	-5.62688	99.99957	99.99254	95.3	4.70%	4.69%
48 CDCl3	-7.31511	-5.62688	99.99957	99.99254	95.2	4.80%	4.79%
49 DMSO	-7.01631	-6.39307	99.99929	99.99795	82.5	17.50%	17.50%
49 Acetone	-7.01631	-6.39307	99.99929	99.99795	92	8.00%	8.00%
49 CDCl3	-7.01631	-6.39307	99.99929	99.99795	88.2	11.80%	11.80%
50 DMSO	N/A	-5.04016	N/A	99.97991	94.6	N/A	5.38%
50 Acetone	N/A	-5.04016	N/A	99.97991	97.8	N/A	2.18%
50 CDCl3	N/A	-5.04016	N/A	99.97991	97.2	N/A	2.78%
51 DMSO	-7.03915	-5.11671	99.99931	99.98235	94	6.00%	5.98%
51 Acetone	-7.03915	-5.11671	99.99931	99.98235	96.4	3.60%	3.58%
51 CDCl3	-7.03915	-5.11671	99.99931	99.98235	96.1	3.90%	3.88%
52 DMSO	-6.82668	N/A	99.99902	N/A	95	5.00%	N/A
52 Acetone	-6.82668	N/A	99.99902	N/A	96.7	3.30%	N/A

52 CDCl3	-6.82668	N/A	99.99902	N/A	97.9	2.10%	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						3.22E3%	1.73E4%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.63%	13.73%

Table 1.9: Convergence results from CAM-B3LYP 6-31G gas phase and how it compares to experimental data.

1.2.5 CAM-B3LYP cc-pVDZ

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-1.44209	-1.44202	91.95016	91.94925	41.7	54.65%	54.65%
2 ethanol	-47180	-47180	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.79589	-0.79568	79.31805	79.31231	44.1	44.40%	44.40%
4 ethanol	-0.83457	-0.83522	80.3693	80.38643	48.3	39.90%	39.92%
5 ethanol	-1.0771	-1.07681	86.04637	86.04047	47.6	44.68%	44.68%
6	16.65988	16.65975	6.03E-11	6.03E-11	6.00E-7	995501.08%	995284.59%
7	16.63449	16.63465	6.29E-11	6.29E-11	1.10E-6	1748554.27%	1749027.02%
8	15.1731	15.17318	7.42E-10	7.42E-10	1.00E-6	134606.45%	134625.03%
9	12.94049	12.93987	3.22E-8	3.23E-8	4.00E-5	124019.30%	123890.88%
10	11.43812	11.43824	4.08E-7	4.07E-7	5.50E-4	134848.11%	134875.36%
11	9.285028	9.285258	1.55E-5	1.55E-5	1.40E-2	90399.79%	90435.01%
12	31.92518	31.92517	3.83E-22	3.83E-22	0	0%	0%
13 CDCl3	-5.38538	-5.38529	99.98878	99.98878	86	13.99%	13.99%
13 DMSO	-5.38538	-5.38529	99.98878	99.98878	63	36.99%	36.99%
13	-5.38538	-5.38529	99.98878	99.98878	80	19.99%	19.99%
14 CDCl3	-3.00444	-3.00452	99.37834	99.37842	3	96.98%	96.98%
14 DMSO	-3.00444	-3.00452	99.37834	99.37842	0	0%	0%

14	-3.00444	-3.00452	99.37834	99.37842	8	91.95%	91.95%
15 CDCl3	-4.36566	-4.36558	99.93726	99.93725	85	14.95%	14.95%
15 DMSO	-4.36566	-4.36558	99.93726	99.93725	99	0.94%	0.94%
15	-4.36566	-4.36558	99.93726	99.93725	89	10.94%	10.94%
16	-3.63341	-3.63391	99.78424	99.78442	80	19.83%	19.83%
17	-5.73128	-5.73104	99.99375	99.99374	91.7	8.29%	8.29%
18	-7.87074	-7.87022	99.99983	99.99983	91.7	8.30%	8.30%
19	-7.06252	-7.06262	99.99934	99.99934	95.8	4.20%	4.20%
20	6.062189	6.062369	0.003576	0.003575	95.3	2664869.24%	2665682.57%
21	-5.20178	-5.20143	99.98471	99.9847	98	1.99%	1.99%
22	-4.9298	-4.92971	99.97579	99.97579	82.1	17.88%	17.88%
23	-4.98166	-4.9818	99.97782	99.97783	91.6	8.38%	8.38%
24	-7.36521	-7.36508	99.9996	99.9996	93.4	6.60%	6.60%
25	7.616598	7.616083	0.000259	0.000259	91.6	35369618.80%	35338852.63%
26	-6.53031	-6.53049	99.99838	99.99838	93.7	6.30%	6.30%
27	-7.92264	-7.92293	99.99985	99.99985	85.2	14.80%	14.80%
28	-7.27203	-7.27158	99.99954	99.99954	88.5	11.50%	11.50%
29	-8.06906	-8.06914	99.99988	99.99988	89.2	10.80%	10.80%
30	-7.7301	-7.72966	99.99979	99.99979	90.8	9.20%	9.20%
31	-4.07982	-4.07944	99.89837	99.8983	93.4	6.50%	6.50%

32	-6.83482	-6.83483	99.99903	99.99903	93.7	6.30%	6.30%
33	-4.63208	-4.63165	99.95999	99.95996	94.6	5.36%	5.36%
34	-5.28489	-5.28551	99.98671	99.98672	93.9	6.09%	6.09%
35	-5.3346	-5.33446	99.98778	99.98778	95.9	4.09%	4.09%
36	-5.38268	-5.3834	99.98873	99.98875	95.6	4.39%	4.39%
37	-6.46194	-6.46209	99.99818	99.99818	97	3.00%	3.00%
38	-5.31314	-5.31312	99.98733	99.98733	97.4	2.59%	2.59%
39	-5.32561	-5.32567	99.98759	99.9876	96.8	3.19%	3.19%
40	-7.28006	-7.28037	99.99954	99.99954	98.1	1.90%	1.90%
41 CDCl3	-3.9841	-3.98406	99.88056	99.88055	40.5	59.45%	59.45%
42 CDCl3	-6.80955	-6.80911	99.99899	99.99899	92.6	7.40%	7.40%
43 DMSO	-6.83998	-6.84048	99.99904	99.99904	94	6.00%	6.00%
43 Acetone	-6.83998	-6.84048	99.99904	99.99904	97.7	2.30%	2.30%
43 CDCl3	-6.83998	-6.84048	99.99904	99.99904	97.8	2.20%	2.20%
44 DMSO	-6.96373	-6.9641	99.99922	99.99922	90.2	9.80%	9.80%
44 Acetone	-6.96373	-6.9641	99.99922	99.99922	93.6	6.40%	6.40%
44 CDCl3	-6.96373	-6.9641	99.99922	99.99922	91.6	8.40%	8.40%
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A
45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A

46 DMSO	-6.88844	-6.88817	99.99911	99.99911	93.7	6.30%	6.30%
46 Acetone	-6.88844	-6.88817	99.99911	99.99911	97.3	2.70%	2.70%
46 CDCl3	-6.88844	-6.88817	99.99911	99.99911	95.7	4.30%	4.30%
47 DMSO	-7.21755	-7.21761	99.99949	99.99949	70.1	29.90%	29.90%
47 Acetone	-7.21755	-7.21761	99.99949	99.99949	87.1	12.90%	12.90%
47 CDCl3	-7.21755	-7.21761	99.99949	99.99949	86.6	13.40%	13.40%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	-6.63687	-6.63654	99.99865	99.99864	82.5	17.50%	17.50%
49 Acetone	-6.63687	-6.63654	99.99865	99.99864	92	8.00%	8.00%
49 CDCl3	-6.63687	-6.63654	99.99865	99.99864	88.2	11.80%	11.80%
50 DMSO	-6.70945	-6.70996	99.9988	99.9988	94.6	5.40%	5.40%
50 Acetone	-6.70945	-6.70996	99.9988	99.9988	97.8	2.20%	2.20%
50 CDCl3	-6.70945	-6.70996	99.9988	99.9988	97.2	2.80%	2.80%
51 DMSO	-6.36086	-6.36044	99.99784	99.99784	94	6.00%	6.00%
51 Acetone	-6.36086	-6.36044	99.99784	99.99784	96.4	3.60%	3.60%
51 CDCl3	-6.36086	-6.36044	99.99784	99.99784	96.1	3.90%	3.90%
52 DMSO	-6.38324	-6.38365	99.99792	99.99792	95	5.00%	5.00%
52 Acetone	-6.38324	-6.38365	99.99792	99.99792	96.7	3.30%	3.30%

52 CDCl3	-6.38324	-6.38365	99.99792	99.99792	97.9	2.10%	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						5.81E3%	5.81E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.05%	14.05%

Table 1.10: Convergence results from CAM-B3LYP cc-pVDZ gas phase and how it compares to experimental data.

1.3 X3LYP gas phase

1.3.1 X3LYP 6-311++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	N/A	N/A	N/A	N/A	41.7	N/A	N/A
2 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
3 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
4 ethanol	N/A	N/A	N/A	N/A	48.3	N/A	N/A
5 ethanol	N/A	N/A	N/A	N/A	47.6	N/A	N/A
6	15.38993	15.3903	5.15E-10	5.14E-10	6.00E-7	116468.68%	116541.93%
7	15.35303	15.35327	5.48E-10	5.48E-10	1.10E-6	200699.48%	200781.48%
8	14.34553	14.34549	3E-9	3E-9	1.00E-6	33194.53%	33192.44%
9	12.11499	12.1147	1.3E-7	1.3E-7	4.00E-5	30685.44%	30670.05%
10	N/A	N/A	N/A	N/A	5.50E-4	N/A	N/A
11	7.020204	7.020576	0.000709	0.000709	1.40E-2	1874.31%	1875.55%
12	31.35945	31.36041	9.95E-22	9.94E-22	0	0%	0%
13 CDCl3	-3.23347	-3.23356	99.57692	99.57698	86	13.63%	13.63%
13 DMSO	-3.23347	-3.23356	99.57692	99.57698	63	36.73%	36.73%
13	-3.23347	-3.23356	99.57692	99.57698	80	19.66%	19.66%
14 CDCl3	-2.1168	-2.11722	97.27518	97.27703	3	96.92%	96.92%

14 DMSO	-2.1168	-2.11722	97.27518	97.27703	0	0%	0%
14	-2.1168	-2.11722	97.27518	97.27703	8	91.78%	91.78%
15 CDCl3	-2.87684	-2.87713	99.23	99.23037	85	14.34%	14.34%
15 DMSO	-2.87684	-2.87713	99.23	99.23037	99	0.23%	0.23%
15	-2.87684	-2.87713	99.23	99.23037	89	10.31%	10.31%
16	-2.64931	-2.64935	98.87326	98.87333	80	19.09%	19.09%
17	-4.12768	-4.1265	99.90625	99.90607	91.7	8.21%	8.21%
18	-5.81855	-5.81827	99.9946	99.9946	91.7	8.30%	8.30%
19	-5.38506	-5.38529	99.98878	99.98878	95.8	4.19%	4.19%
20	6.575556	6.575672	0.001503	0.001502	95.3	6342033.17%	6343278.59%
21	-4.50639	-4.50615	99.95053	99.95051	98	1.95%	1.95%
22	-3.47789	-3.47766	99.71961	99.7195	82.1	17.67%	17.67%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-5.38199	-5.38152	99.98872	99.98871	93.4	6.59%	6.59%
25	7.09919	7.099642	0.000621	0.00062	91.6	14760933.40%	14772228.50%
26	-5.1345	-5.13491	99.98287	99.98288	93.7	6.28%	6.28%
27	-3.9601	-3.96021	99.87562	99.87564	85.2	14.69%	14.69%
28	-3.74516	-3.7456	99.82128	99.82142	88.5	11.34%	11.34%
29	-4.62326	-4.62349	99.95938	99.9594	89.2	10.76%	10.76%
30	-3.7655	-3.76568	99.82731	99.82736	90.8	9.04%	9.04%

31	-4.81961	-4.81927	99.97084	99.97083	93.4	6.57%	6.57%
32	-5.23497	-5.23468	99.98554	99.98553	93.7	6.29%	6.29%
33	-6.4262	-6.42632	99.99807	99.99807	94.6	5.40%	5.40%
34	-4.24105	-4.24134	99.92258	99.92261	93.9	6.03%	6.03%
35	-4.58067	-4.58082	99.95636	99.95637	95.9	4.06%	4.06%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-2.92385	-2.92357	99.28835	99.28801	40.5	59.21%	59.21%
42 CDCl3	-4.523	-4.52309	99.95189	99.9519	92.6	7.36%	7.36%
43 DMSO	-5.4262	-5.4267	99.98953	99.98954	94	5.99%	5.99%
43 Acetone	-5.4262	-5.4267	99.98953	99.98954	97.7	2.29%	2.29%
43 CDCl3	-5.4262	-5.4267	99.98953	99.98954	97.8	2.19%	2.19%
44 DMSO	-6.76857	-6.76894	99.99892	99.99892	90.2	9.80%	9.80%
44 Acetone	-6.76857	-6.76894	99.99892	99.99892	93.6	6.40%	6.40%
44 CDCl3	-6.76857	-6.76894	99.99892	99.99892	91.6	8.40%	8.40%
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A

45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 DMSO	-5.49022	-5.49071	99.9906	99.99061	93.7	6.29%	6.29%
46 Acetone	-5.49022	-5.49071	99.9906	99.99061	97.3	2.69%	2.69%
46 CDCl3	-5.49022	-5.49071	99.9906	99.99061	95.7	4.29%	4.29%
47 DMSO	-6.72247	-6.72188	99.99883	99.99883	70.1	29.90%	29.90%
47 Acetone	-6.72247	-6.72188	99.99883	99.99883	87.1	12.90%	12.90%
47 CDCl3	-6.72247	-6.72188	99.99883	99.99883	86.6	13.40%	13.40%
48 DMSO	10.26258	10.26229	2.97E-6	2.97E-6	90.7	3056043777.00%	3054526001.80%
48 Acetone	10.26258	10.26229	2.97E-6	2.97E-6	95.3	3211036079.47%	3209441327.80%
48 CDCl3	10.26258	10.26229	2.97E-6	2.97E-6	95.2	3207666681.59%	3206073603.32%
49 DMSO	-6.29639	-6.29643	99.99759	99.99759	82.5	17.50%	17.50%
49 Acetone	-6.29639	-6.29643	99.99759	99.99759	92	8.00%	8.00%
49 CDCl3	-6.29639	-6.29643	99.99759	99.99759	88.2	11.80%	11.80%
50 DMSO	-5.44316	-5.44302	99.98983	99.98983	94.6	5.39%	5.39%
50 Acetone	-5.44316	-5.44302	99.98983	99.98983	97.8	2.19%	2.19%
50 CDCl3	-5.44316	-5.44302	99.98983	99.98983	97.2	2.79%	2.79%
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95	N/A	N/A

52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.67E6%	1.67E6%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						13.80%	13.80%

Table 1.11: Convergence results from X3LYP 6-311++G gas phase and how it compares to experimental data.

1.3.2 X3LYP 6-31++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	N/A	N/A	N/A	N/A	41.7	N/A	N/A
2 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
3 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
4 ethanol	N/A	N/A	N/A	N/A	48.3	N/A	N/A
5 ethanol	N/A	N/A	N/A	N/A	47.6	N/A	N/A
6	16.19197	16.19226	1.33E-10	1.33E-10	6.00E-7	451628.58%	451845.51%
7	15.8802	15.87976	2.25E-10	2.25E-10	1.10E-6	489044.74%	488676.80%
8	14.85333	14.85315	1.27E-9	1.27E-9	1.00E-6	78394.57%	78370.80%
9	12.55081	12.55019	6.22E-8	6.23E-8	4.00E-5	64170.69%	64103.54%
10	10.44425	10.44364	2.18E-6	2.19E-6	5.50E-4	25086.53%	25060.47%
11	7.422348	7.42281	0.00036	0.000359	1.40E-2	3793.89%	3796.92%
12	31.77367	31.77332	4.95E-22	4.95E-22	0	0%	0%
13 CDCl3	-5.10871	-5.10855	99.98211	99.9821	86	13.98%	13.98%
13 DMSO	-5.10871	-5.10855	99.98211	99.9821	63	36.99%	36.99%
13	-5.10871	-5.10855	99.98211	99.9821	80	19.99%	19.99%
14 CDCl3	-2.54244	-2.5433	98.65338	98.6553	3	96.96%	96.96%
14 DMSO	-2.54244	-2.5433	98.65338	98.6553	0	0%	0%

14	-2.54244	-2.5433	98.65338	98.6553	8	91.89%	91.89%
15 CDCl3	N/A	N/A	N/A	N/A	85	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99	N/A	N/A
15	N/A	N/A	N/A	N/A	89	N/A	N/A
16	-3.39951	-3.39985	99.68005	99.68023	80	19.74%	19.74%
17	-4.78556	-4.78476	99.96912	99.96908	91.7	8.27%	8.27%
18	-6.56813	-6.56751	99.99848	99.99848	91.7	8.30%	8.30%
19	-6.01891	-6.01907	99.99615	99.99615	95.8	4.20%	4.20%
20	6.435621	6.435737	0.001903	0.001903	95.3	5007109.73%	5008093.00%
21	-5.52729	-5.5271	99.99117	99.99117	98	1.99%	1.99%
22	-4.21129	-4.21184	99.91859	99.91866	82.1	17.83%	17.83%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-6.14045	-6.14018	99.99687	99.99687	93.4	6.60%	6.60%
25	7.094581	7.09525	0.000625	0.000625	91.6	14646474.73%	14663042.40%
26	-5.87526	-5.87537	99.9951	99.9951	93.7	6.30%	6.30%
27	-4.74204	-4.74209	99.96677	99.96677	85.2	14.77%	14.77%
28	-4.53926	-4.54003	99.9532	99.95326	88.5	11.46%	11.46%
29	-5.30938	-5.30999	99.98725	99.98726	89.2	10.79%	10.79%
30	-4.28893	-4.2884	99.92859	99.92852	90.8	9.14%	9.14%
31	-5.59619	-5.5955	99.99214	99.99214	93.4	6.59%	6.59%

32	-4.20501	-4.20431	99.91772	99.91762	93.7	6.22%	6.22%
33	-7.23238	-7.23205	99.9995	99.9995	94.6	5.40%	5.40%
34	-5.11189	-5.11169	99.9822	99.9822	93.9	6.08%	6.08%
35	-5.12795	-5.12801	99.98268	99.98268	95.9	4.08%	4.08%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-3.81691	-3.81651	99.84165	99.84154	40.5	59.44%	59.44%
42 CDCl3	-5.59131	-5.59174	99.99208	99.99208	92.6	7.39%	7.39%
43 DMSO	-6.18068	-6.18034	99.99707	99.99707	94	6.00%	6.00%
43 Acetone	-6.18068	-6.18034	99.99707	99.99707	97.7	2.30%	2.30%
43 CDCl3	-6.18068	-6.18034	99.99707	99.99707	97.8	2.20%	2.20%
44 DMSO	-7.44171	-7.44101	99.99965	99.99965	90.2	9.80%	9.80%
44 Acetone	-7.44171	-7.44101	99.99965	99.99965	93.6	6.40%	6.40%
44 CDCl3	-7.44171	-7.44101	99.99965	99.99965	91.6	8.40%	8.40%
45 DMSO	-6.87033	-6.86997	99.99909	99.99909	94.6	5.40%	5.40%
45Acetone	-6.87033	-6.86997	99.99909	99.99909	99.3	0.70%	0.70%
45 CDCl3	-6.87033	-6.86997	99.99909	99.99909	97.3	2.70%	2.70%

46 DMSO	-6.06526	-6.06551	99.99644	99.99644	93.7	6.30%	6.30%
46 Acetone	-6.06526	-6.06551	99.99644	99.99644	97.3	2.70%	2.70%
46 CDCl3	-6.06526	-6.06551	99.99644	99.99644	95.7	4.30%	4.30%
47 DMSO	-6.66543	-6.66603	99.99871	99.99871	70.1	29.90%	29.90%
47 Acetone	-6.66543	-6.66603	99.99871	99.99871	87.1	12.90%	12.90%
47 CDCl3	-6.66543	-6.66603	99.99871	99.99871	86.6	13.40%	13.40%
48 DMSO	10.25694	10.25727	3E-6	2.99E-6	90.7	3027032588.61%	3028737444.71%
48 Acetone	10.25694	10.25727	3E-6	2.99E-6	95.3	3180553540.85%	3182344861.53%
48 CDCl3	10.25694	10.25727	3E-6	2.99E-6	95.2	3177216128.84%	3179005569.86%
49 DMSO	-7.00436	-7.00489	99.99927	99.99927	82.5	17.50%	17.50%
49 Acetone	-7.00436	-7.00489	99.99927	99.99927	92	8.00%	8.00%
49 CDCl3	-7.00436	-7.00489	99.99927	99.99927	88.2	11.80%	11.80%
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A

52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.71E6%	1.71E6%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.21%	14.21%

Table 1.12: Convergence results from X3LYP 6-31++G gas phase and how it compares to experimental data.

1.3.3 X3LYP 6-31+G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.55917	-0.55848	71.99881	71.9754	41.7	42.08%	42.06%
2 ethanol	-47175.3	-47175.3	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.16356	-0.16378	56.86245	56.87158	44.1	22.44%	22.46%
4 ethanol	-0.11444	-0.11421	54.8171	54.8073	48.3	11.89%	11.87%
5 ethanol	-0.47944	-0.47942	69.20548	69.20465	47.6	31.22%	31.22%
6	16.74532	16.74446	5.22E-11	5.22E-11	6.00E-7	1150057.33%	1148392.15%
7	15.92119	15.92117	2.1E-10	2.1E-10	1.10E-6	524104.09%	524090.00%
8	14.98971	14.98995	1.01E-9	1.01E-9	1.00E-6	98726.67%	98766.24%
9	12.63157	12.63177	5.43E-8	5.43E-8	4.00E-5	73562.87%	73587.66%
10	10.53299	10.53212	1.88E-6	1.88E-6	5.50E-4	29158.54%	29115.78%
11	7.586543	7.585962	0.000272	0.000273	1.40E-2	5038.29%	5033.26%
12	31.87085	31.87058	4.2E-22	4.2E-22	0	0%	0%
13 CDCl3	-5.31639	-5.31626	99.9874	99.9874	86	13.99%	13.99%
13 DMSO	-5.31639	-5.31626	99.9874	99.9874	63	36.99%	36.99%
13	-5.31639	-5.31626	99.9874	99.9874	80	19.99%	19.99%
14 CDCl3	-2.49618	-2.49623	98.54553	98.54567	3	96.96%	96.96%
14 DMSO	-2.49618	-2.49623	98.54553	98.54567	0	0%	0%

14	-2.49618	-2.49623	98.54553	98.54567	8	91.88%	91.88%
15 CDCl3	-3.44664	-3.44691	99.70446	99.70459	85	14.75%	14.75%
15 DMSO	-3.44664	-3.44691	99.70446	99.70459	99	0.71%	0.71%
15	-3.44664	-3.44691	99.70446	99.70459	89	10.74%	10.74%
16	-3.36105	-3.36094	99.65865	99.65859	80	19.73%	19.73%
17	-4.77264	-4.77284	99.96844	99.96845	91.7	8.27%	8.27%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-5.97708	-5.97703	99.99587	99.99587	95.8	4.20%	4.20%
20	N/A	N/A	N/A	N/A	95.3	N/A	N/A
21	-5.50236	-5.50138	99.9908	99.99078	98	1.99%	1.99%
22	-4.14656	-4.14658	99.90919	99.9092	82.1	17.83%	17.83%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-6.09928	-6.09939	99.99664	99.99664	93.4	6.60%	6.60%
25	N/A	N/A	N/A	N/A	91.6	N/A	N/A
26	-5.81824	-5.81827	99.9946	99.9946	93.7	6.29%	6.29%
27	-4.85901	-4.85881	99.97272	99.97271	85.2	14.78%	14.78%
28	-4.48672	-4.48732	99.94886	99.94891	88.5	11.45%	11.45%
29	-5.28301	-5.28363	99.98667	99.98668	89.2	10.79%	10.79%
30	-4.22794	-4.22816	99.92084	99.92087	90.8	9.13%	9.13%
31	-5.54859	-5.54844	99.99149	99.99148	93.4	6.59%	6.59%

32	-4.15782	-4.15788	99.9109	99.91091	93.7	6.22%	6.22%
33	-7.20966	-7.20883	99.99949	99.99948	94.6	5.40%	5.40%
34	N/A	N/A	N/A	N/A	93.9	N/A	N/A
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-3.70521	-3.70482	99.80883	99.8087	40.5	59.42%	59.42%
42 CDCl3	-5.53327	-5.53338	99.99126	99.99127	92.6	7.39%	7.39%
43 DMSO	-6.56376	-6.56375	99.99847	99.99847	94	6.00%	6.00%
43 Acetone	-6.56376	-6.56375	99.99847	99.99847	97.7	2.30%	2.30%
43 CDCl3	-6.56376	-6.56375	99.99847	99.99847	97.8	2.20%	2.20%
44 DMSO	-7.53852	-7.53953	99.9997	99.99971	90.2	9.80%	9.80%
44 Acetone	-7.53852	-7.53953	99.9997	99.99971	93.6	6.40%	6.40%
44 CDCl3	-7.53852	-7.53953	99.9997	99.99971	91.6	8.40%	8.40%
45 DMSO	-6.06375	-6.06362	99.99643	99.99643	94.6	5.40%	5.40%
45Acetone	-6.06375	-6.06362	99.99643	99.99643	99.3	0.70%	0.70%
45 CDCl3	-6.06375	-6.06362	99.99643	99.99643	97.3	2.70%	2.70%

46 DMSO	-6.20586	-6.20544	99.99719	99.99719	93.7	6.30%	6.30%
46 Acetone	-6.20586	-6.20544	99.99719	99.99719	97.3	2.70%	2.70%
46 CDCl3	-6.20586	-6.20544	99.99719	99.99719	95.7	4.30%	4.30%
47 DMSO	-6.72602	-6.72502	99.99883	99.99883	70.1	29.90%	29.90%
47 Acetone	-6.72602	-6.72502	99.99883	99.99883	87.1	12.90%	12.90%
47 CDCl3	-6.72602	-6.72502	99.99883	99.99883	86.6	13.40%	13.40%
48 DMSO	-6.35946	-6.35918	99.99784	99.99783	90.7	9.30%	9.30%
48 Acetone	-6.35946	-6.35918	99.99784	99.99783	95.3	4.70%	4.70%
48 CDCl3	-6.35946	-6.35918	99.99784	99.99783	95.2	4.80%	4.80%
49 DMSO	-7.00481	-7.00489	99.99927	99.99927	82.5	17.50%	17.50%
49 Acetone	-7.00481	-7.00489	99.99927	99.99927	92	8.00%	8.00%
49 CDCl3	-7.00481	-7.00489	99.99927	99.99927	88.2	11.80%	11.80%
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	-5.86358	-5.86408	99.995	99.995	94	6.00%	6.00%
51 Acetone	-5.86358	-5.86408	99.995	99.995	96.4	3.60%	3.60%
51 CDCl3	-5.86358	-5.86408	99.995	99.995	96.1	3.90%	3.90%
52 DMSO	-5.83071	-5.83082	99.99471	99.99471	95	4.99%	4.99%
52 Acetone	-5.83071	-5.83082	99.99471	99.99471	96.7	3.29%	3.29%

52 CDCl3	-5.83071	-5.83082	99.99471	99.99471	97.9	2.09%	2.09%
Mean Error of Theoretical Calculation of Gas Phase vs literature						2.99E2%	2.98E2%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						13.74%	13.74%

Table 1.13: Convergence results from X3LYP 6-31+G gas phase and how it compares to experimental data.

1.3.4 X3LYP 6-31G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.78619	-0.78627	79.04814	79.05025	41.7	47.25%	47.25%
2 ethanol	-47173.6	-47173.6	N/A	N/A	44.1	N/A	N/A
3 ethanol	-1.49187	-1.49159	92.55096	92.54767	44.1	52.35%	52.35%
4 ethanol	-0.32237	-0.32254	63.28505	63.29164	48.3	23.68%	23.69%
5 ethanol	-0.59544	-0.59551	73.21687	73.21918	47.6	34.99%	34.99%
6	17.49856	17.49873	1.46E-11	1.46E-11	6.00E-7	4104334.30%	4105517.83%
7	17.47171	17.47112	1.53E-11	1.53E-11	1.10E-6	7191091.22%	7183925.37%
8	15.81697	15.817	2.5E-10	2.5E-10	1.00E-6	399537.79%	399559.74%
9	13.54364	13.54354	1.16E-8	1.16E-8	4.00E-5	343653.65%	343595.82%
10	12.01681	12.01743	1.53E-7	1.53E-7	5.50E-4	358513.81%	358894.89%
11	9.314974	9.314751	1.47E-5	1.47E-5	1.40E-2	95094.78%	95058.91%
12	33.17203	33.17203	4.66E-23	4.66E-23	0	0.00%	0.00%
13 CDCl3	-5.40284	-5.40286	99.98911	99.98911	86	13.99%	13.99%
13 DMSO	-5.40284	-5.40286	99.98911	99.98911	63	36.99%	36.99%
13	-5.40284	-5.40286	99.98911	99.98911	80	19.99%	19.99%
14 CDCl3	-2.57797	-2.57844	98.73082	98.7318	3	96.96%	96.96%
14 DMSO	-2.57797	-2.57844	98.73082	98.7318	0	0.00%	0.00%

14	-2.57797	-2.57844	98.73082	98.7318	8	91.90%	91.90%
15 CDCl3	N/A	N/A	N/A	N/A	85	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99	N/A	N/A
15	N/A	N/A	N/A	N/A	89	N/A	N/A
16	-3.39043	-3.39106	99.67512	99.67546	80	19.74%	19.74%
17	-5.58725	-5.58734	99.99202	99.99203	91.7	8.29%	8.29%
18	-7.47489	-7.47489	99.99967	99.99967	91.7	8.30%	8.30%
19	-5.99799	-5.99836	99.99601	99.99602	95.8	4.20%	4.20%
20	6.539075	6.538649	0.001598	0.001599	95.3	5963067.18%	5958782.62%
21	-4.96957	-4.96988	99.97737	99.97738	98	1.98%	1.98%
22	-4.48335	-4.48356	99.94856	99.94858	82.1	17.86%	17.86%
23	-4.66042	-4.65989	99.96186	99.96182	91.6	8.37%	8.37%
24	-6.57544	-6.57567	99.9985	99.9985	93.4	6.60%	6.60%
25	7.692021	7.692011	0.000228	0.000228	91.6	40174688.57%	40174060.22%
26	-5.89894	-5.89859	99.99529	99.99529	93.7	6.30%	6.30%
27	-7.2585	-7.2584	99.99953	99.99953	85.2	14.80%	14.80%
28	-4.30761	-4.30723	99.9308	99.93076	88.5	11.44%	11.44%
29	-7.6331	-7.63303	99.99975	99.99975	89.2	10.80%	10.80%
30	-6.40519	-6.40499	99.998	99.998	90.8	9.20%	9.20%
31	-5.62221	-5.62186	99.99248	99.99248	93.4	6.59%	6.59%

32	-4.24815	-4.24761	99.9235	99.92343	93.7	6.23%	6.23%
33	-4.506	-4.50615	99.95049	99.95051	94.6	5.35%	5.35%
34	-4.88477	-4.88516	99.97388	99.9739	93.9	6.08%	6.08%
35	-5.04613	-5.04643	99.98011	99.98012	95.9	4.08%	4.08%
36	-4.94447	-4.94477	99.97639	99.9764	95.6	4.38%	4.38%
37	-5.91921	-5.91867	99.99545	99.99544	97	3.00%	3.00%
38	-4.8049	-4.80484	99.97011	99.97011	97.4	2.57%	2.57%
39	-5.24659	-5.24598	99.98582	99.98581	96.8	3.19%	3.19%
40	-6.25764	-6.25752	99.99743	99.99743	98.1	1.90%	1.90%
41 CDCl3	-4.1211	-4.12023	99.90521	99.90507	40.5	59.46%	59.46%
42 CDCl3	-6.19581	-6.1954	99.99715	99.99714	92.6	7.40%	7.40%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-7.01762	-7.01807	99.99929	99.99929	90.2	9.80%	9.80%
44 Acetone	-7.01762	-7.01807	99.99929	99.99929	93.6	6.40%	6.40%
44 CDCl3	-7.01762	-7.01807	99.99929	99.99929	91.6	8.40%	8.40%
45 DMSO	-6.04125	-6.04166	99.9963	99.9963	94.6	5.40%	5.40%
45Acetone	-6.04125	-6.04166	99.9963	99.9963	99.3	0.70%	0.70%
45 CDCl3	-6.04125	-6.04166	99.9963	99.9963	97.3	2.70%	2.70%

46 DMSO	-5.92365	-5.92369	99.99548	99.99548	93.7	6.30%	6.30%
46 Acetone	-5.92365	-5.92369	99.99548	99.99548	97.3	2.70%	2.70%
46 CDCl3	-5.92365	-5.92369	99.99548	99.99548	95.7	4.30%	4.30%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	-6.12007	-6.1201	99.99676	99.99676	90.7	9.30%	9.30%
48 Acetone	-6.12007	-6.1201	99.99676	99.99676	95.3	4.70%	4.70%
48 CDCl3	-6.12007	-6.1201	99.99676	99.99676	95.2	4.80%	4.80%
49 DMSO	N/A	-6.87374	N/A	99.99909	82.5	N/A	17.50%
49 Acetone	N/A	-6.87374	N/A	99.99909	92	N/A	8.00%
49 CDCl3	N/A	-6.87374	N/A	99.99909	88.2	N/A	11.80%
50 DMSO	N/A	-5.82643	N/A	99.99467	94.6	N/A	5.39%
50 Acetone	N/A	-5.82643	N/A	99.99467	97.8	N/A	2.19%
50 CDCl3	N/A	-5.82643	N/A	99.99467	97.2	N/A	2.79%
51 DMSO	N/A	-5.82203	N/A	99.99464	94	N/A	5.99%
51 Acetone	N/A	-5.82203	N/A	99.99464	96.4	N/A	3.59%
51 CDCl3	N/A	-5.82203	N/A	99.99464	96.1	N/A	3.89%
52 DMSO	N/A	-5.92369	N/A	99.99548	95	N/A	5.00%
52 Acetone	N/A	-5.92369	N/A	99.99548	96.7	N/A	3.30%

52 CDCl3	N/A	-5.92369	N/A	99.99548	97.9	N/A	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.05E4%	8.62E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						15.03%	13.22%

Table 1.14: Convergence results from X3LYP 6-31+G gas phase and how it compares to experimental data.

1.3.5 X3LYP cc-pVDZ

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.84433	-0.844	80.62814	80.61931	41.7	48.28%	48.28%
2 ethanol	-47176.4	-47176.4	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.47322	-0.47251	68.98123	68.95564	44.1	36.07%	36.05%
4 ethanol	N/A	N/A	N/A	N/A	48.3	N/A	N/A
5 ethanol	-0.29686	-0.29744	62.27818	62.30128	47.6	23.57%	23.60%
6	16.5626	16.56249	7.1E-11	7.1E-11	6.00E-7	844654.60%	844494.59%
7	16.50002	16.50036	7.89E-11	7.89E-11	1.10E-6	1393289.81%	1394091.75%
8	14.92333	14.92343	1.13E-9	1.13E-9	1.00E-6	88245.39%	88260.64%
9	12.81103	12.81123	4.01E-8	4.01E-8	4.00E-5	99642.55%	99677.68%
10	11.27764	11.27823	5.34E-7	5.34E-7	5.50E-4	102808.41%	102911.18%
11	9.020097	9.019822	2.42E-5	2.42E-5	1.40E-2	57752.54%	57725.62%
12	31.75963	31.75951	5.06E-22	5.06E-22	0	0.00%	0.00%
13 CDCl3	-5.75034	-5.74987	99.99394	99.99394	86	13.99%	13.99%
13 DMSO	-5.75034	-5.74987	99.99394	99.99394	63	37.00%	37.00%
13	-5.75034	-5.74987	99.99394	99.99394	80	20.00%	20.00%
14 CDCl3	-3.27262	-3.27246	99.60388	99.60377	3	96.99%	96.99%
14 DMSO	-3.27262	-3.27246	99.60388	99.60377	0	0.00%	0.00%

14	-3.27262	-3.27246	99.60388	99.60377	8	91.97%	91.97%
15 CDCl3	-4.46386	-4.4641	99.94684	99.94687	85	14.95%	14.95%
15 DMSO	-4.46386	-4.4641	99.94684	99.94687	99	0.95%	0.95%
15	-4.46386	-4.4641	99.94684	99.94687	89	10.95%	10.95%
16	-3.72794	-3.72803	99.81602	99.81605	80	19.85%	19.85%
17	-5.79934	-5.79944	99.99443	99.99443	91.7	8.29%	8.29%
18	-7.87305	-7.87273	99.99983	99.99983	91.7	8.30%	8.30%
19	-6.90829	-6.90825	99.99914	99.99914	95.8	4.20%	4.20%
20	5.77612	5.776225	0.005797	0.005796	95.3	1643787.12%	1644078.61%
21	-5.52577	-5.52585	99.99115	99.99115	98	1.99%	1.99%
22	-4.93731	-4.93724	99.9761	99.9761	82.1	17.88%	17.88%
23	-5.07099	-5.07153	99.98093	99.98095	91.6	8.38%	8.38%
24	-7.34474	-7.34437	99.99959	99.99959	93.4	6.60%	6.60%
25	7.139275	7.139803	0.00058	0.000579	91.6	15794882.10%	15808971.99%
26	-6.58668	-6.58697	99.99853	99.99853	93.7	6.30%	6.30%
27	-7.88437	-7.88403	99.99984	99.99984	85.2	14.80%	14.80%
28	-7.49923	-7.49937	99.99968	99.99968	88.5	11.50%	11.50%
29	-8.27757	-8.27811	99.99992	99.99992	89.2	10.80%	10.80%
30	-4.86724	-4.86759	99.9731	99.97311	90.8	9.18%	9.18%
31	-6.27485	-6.27572	99.9975	99.99751	93.4	6.60%	6.60%

32	-4.81167	-4.81174	99.97045	99.97046	93.7	6.27%	6.27%
33	-4.97307	-4.97364	99.9775	99.97752	94.6	5.38%	5.38%
34	-5.65444	-5.65449	99.99288	99.99288	93.9	6.09%	6.09%
35	-5.746	-5.7461	99.9939	99.9939	95.9	4.09%	4.09%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	-6.768	-6.76769	99.99891	99.99891	97	3.00%	3.00%
38	-5.54571	-5.54593	99.99145	99.99145	97.4	2.59%	2.59%
39	-5.89031	-5.89043	99.99522	99.99522	96.8	3.20%	3.20%
40	-7.67897	-7.67946	99.99977	99.99977	98.1	1.90%	1.90%
41 CDCl3	-4.28508	-4.28526	99.92812	99.92814	40.5	59.47%	59.47%
42 CDCl3	-6.76721	-6.76706	99.99891	99.99891	92.6	7.40%	7.40%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-7.4703	-7.47113	99.99967	99.99967	90.2	9.80%	9.80%
44 Acetone	-7.4703	-7.47113	99.99967	99.99967	93.6	6.40%	6.40%
44 CDCl3	-7.4703	-7.47113	99.99967	99.99967	91.6	8.40%	8.40%
45 DMSO	-8.36693	-8.36658	99.99993	99.99993	94.6	5.40%	5.40%
45Acetone	-8.36693	-8.36658	99.99993	99.99993	99.3	0.70%	0.70%
45 CDCl3	-8.36693	-8.36658	99.99993	99.99993	97.3	2.70%	2.70%

46 DMSO	-7.75029	-7.75037	99.99979	99.99979	93.7	6.30%	6.30%
46 Acetone	-7.75029	-7.75037	99.99979	99.99979	97.3	2.70%	2.70%
46 CDCl3	-7.75029	-7.75037	99.99979	99.99979	95.7	4.30%	4.30%
47 DMSO	-7.49099	-7.49121	99.99968	99.99968	70.1	29.90%	29.90%
47 Acetone	-7.49099	-7.49121	99.99968	99.99968	87.1	12.90%	12.90%
47 CDCl3	-7.49099	-7.49121	99.99968	99.99968	86.6	13.40%	13.40%
48 DMSO	-7.34692	-7.34688	99.99959	99.99959	90.7	9.30%	9.30%
48 Acetone	-7.34692	-7.34688	99.99959	99.99959	95.3	4.70%	4.70%
48 CDCl3	-7.34692	-7.34688	99.99959	99.99959	95.2	4.80%	4.80%
49 DMSO	-7.08294	-7.08333	99.99936	99.99936	82.5	17.50%	17.50%
49 Acetone	-7.08294	-7.08333	99.99936	99.99936	92	8.00%	8.00%
49 CDCl3	-7.08294	-7.08333	99.99936	99.99936	88.2	11.80%	11.80%
50 DMSO	-7.67418	-7.67444	99.99977	99.99977	94.6	5.40%	5.40%
50 Acetone	-7.67418	-7.67444	99.99977	99.99977	97.8	2.20%	2.20%
50 CDCl3	-7.67418	-7.67444	99.99977	99.99977	97.2	2.80%	2.80%
51 DMSO	-7.40303	-7.40336	99.99963	99.99963	94	6.00%	6.00%
51 Acetone	-7.40303	-7.40336	99.99963	99.99963	96.4	3.60%	3.60%
51 CDCl3	-7.40303	-7.40336	99.99963	99.99963	96.1	3.90%	3.90%
52 DMSO	-6.90678	-6.907	99.99914	99.99914	95	5.00%	5.00%
52 Acetone	-6.90678	-6.907	99.99914	99.99914	96.7	3.30%	3.30%

52 CDCl3	-6.90678	-6.907	99.99914	99.99914	97.9	2.10%	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						2.78E3%	2.78E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.84%	12.84%

Table 1.15: Convergence results from X3LYP cc-pVDZ gas phase and how it compares to experimental data.

1.4 M05 gas phase

1.4.1 M05 6-311++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.22604	-0.2259	59.43003	59.42435155	41.7	29.83%	29.83%
2 ethanol	-47184.8	-47184.8	N/A	N/A	44.1	N/A	N/A
3 ethanol	3.400125	3.400474	0.319621	0.319433559	44.1	13697.58%	13705.69%
4 ethanol	0.434594	0.434864	32.43175	32.42174737	48.3	48.93%	48.97%
5 ethanol	-0.21182	-0.21147	58.84938	58.83527997	47.6	19.12%	19.10%
6	17.79554	17.79617	8.85E-12	8.84306E-12	6.00E-7	6777712.15%	6784884.30%
7	17.91287	17.91351	7.26E-12	7.25322E-12	1.10E-6	15149100.55%	15165573.35%
8	17.01456	17.01492	3.31E-11	3.3086E-11	1.00E-6	3020510.38%	3022323.26%
9	14.90563	14.90523	1.17E-9	1.16705E-9	4.00E-5	3429662.97%	3427348.13%
10	12.98786	12.98819	2.97E-8	2.97323E-8	5.50E-4	1848713.05%	1849737.65%
11	9.457952	9.457823	1.16E-5	1.15541E-5	1.40E-2	121095.55%	121069.17%
12	35.35784	35.35765	1.16E-24	1.16238E-24	0	0%	0%
13 CDCl3	-1.20548	-1.20545	88.45227	88.45170125	86	2.77%	2.77%
13 DMSO	-1.20548	-1.20545	88.45227	88.45170125	63	28.78%	28.77%
13	-1.20548	-1.20545	88.45227	88.45170125	80	9.56%	9.56%
14 CDCl3	0.793317	0.793172	20.7533	20.75733276	3	85.54%	85.55%

14 DMSO	0.793317	0.793172	20.7533	20.75733276	0	0.00%	0.00%
14	0.793317	0.793172	20.7533	20.75733276	8	61.45%	61.46%
15 CDCl3	0.040698	0.040788	48.28228	48.27846962	85	76.05%	76.06%
15 DMSO	0.040698	0.040788	48.28228	48.27846962	99	105.04%	105.06%
15	0.040698	0.040788	48.28228	48.27846962	89	84.33%	84.35%
16	N/A	N/A	N/A	N/A	80	N/A	N/A
17	N/A	N/A	N/A	N/A	91.7	N/A	N/A
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-1.40968	-1.40939	91.53553	91.53174008	95.8	4.66%	4.66%
20	8.838835	8.838471	3.29E-5	3.28872E-5	95.3	289956239.84%	289778107.38%
21	-0.93746	-0.9375	82.96732	82.96818883	98	18.12%	18.12%
22	0.414107	0.414156	33.19454	33.19269347	82.1	147.33%	147.34%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-1.84933	-1.8499	95.78479	95.78862992	93.4	2.49%	2.49%
25	10.01665	10.01693	4.5E-6	4.49398E-6	91.6	2037302618.97%	2038283115.51%
26	-1.5773	-1.57693	93.48658	93.48280403	93.7	0.23%	0.23%
27	-0.07428	-0.07467	53.1323	53.14879855	85.2	60.35%	60.30%
28	-0.39292	-0.39282	66.00729	66.003467	88.5	34.08%	34.08%
29	-0.9084	-0.90801	82.26247	82.25269937	89.2	8.43%	8.45%
30	-2.10293	-2.10278	97.21237	97.21171448	90.8	6.60%	6.60%

31	-1.24932	-1.24937	89.18725	89.18815628	93.4	4.72%	4.72%
32	0.009227	0.008785	49.61043	49.62906902	93.7	88.87%	88.80%
33	-2.81542	-2.81564	99.14654	99.14685035	94.6	4.59%	4.59%
34	-0.76869	-0.76807	78.55431	78.536715	93.9	19.54%	19.56%
35	-0.32582	-0.32568	63.42021	63.41466675	95.9	51.21%	51.23%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	0.402233	0.402861	33.64075	33.61707209	40.5	20.39%	20.47%
42 CDCl3	-1.72781	-1.72816	94.87366	94.87655931	92.6	2.40%	2.40%
43 DMSO	-1.62839	-1.62776	93.99273	93.98669599	94	0.01%	0.01%
43 Acetone	-1.62839	-1.62776	93.99273	93.98669599	97.7	3.94%	3.95%
43 CDCl3	-1.62839	-1.62776	93.99273	93.98669599	97.8	4.05%	4.06%
44 DMSO	-3.68589	-3.68599	99.8025	99.80253664	90.2	9.62%	9.62%
44 Acetone	-3.68589	-3.68599	99.8025	99.80253664	93.6	6.21%	6.21%
44 CDCl3	-3.68589	-3.68599	99.8025	99.80253664	91.6	8.22%	8.22%
45 DMSO	-2.38835	-2.3883	98.26007	98.25991713	94.6	3.72%	3.72%
45Acetone	-2.38835	-2.3883	98.26007	98.25991713	99.3	1.06%	1.06%

45 CDCl3	-2.38835	-2.3883	98.26007	98.25991713	97.3	0.98%	0.98%
46 DMSO	-1.30034	-1.29957	89.99072	89.97898593	93.7	4.12%	4.14%
46 Acetone	-1.30034	-1.29957	89.99072	89.97898593	97.3	8.12%	8.14%
46 CDCl3	-1.30034	-1.29957	89.99072	89.97898593	95.7	6.34%	6.36%
47 DMSO	-2.86619	-2.86646	99.21612	99.21648402	70.1	29.35%	29.35%
47 Acetone	-2.86619	-2.86646	99.21612	99.21648402	87.1	12.21%	12.21%
47 CDCl3	-2.86619	-2.86646	99.21612	99.21648402	86.6	12.72%	12.72%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-1.58227	-1.58258	93.53755	93.54067587	94.6	1.14%	1.13%
50 Acetone	-1.58227	-1.58258	93.53755	93.54067587	97.8	4.56%	4.55%
50 CDCl3	-1.58227	-1.58258	93.53755	93.54067587	97.2	3.92%	3.91%
51 DMSO	-1.94323	-1.94277	96.3806	96.37785357	94	2.47%	2.47%
51 Acetone	-1.94323	-1.94277	96.3806	96.37785357	96.4	0.02%	0.02%
51 CDCl3	-1.94323	-1.94277	96.3806	96.37785357	96.1	0.29%	0.29%
52 DMSO	N/A	N/A	N/A	N/A	95	N/A	N/A

52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						4.00E5%	4.00E5%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						22.97%	22.97%

Table 1.16: Convergence results from M05 6-311++G gas phase and how it compares to experimental data.

1.4.2 M05 6-31++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.17155	-0.17131	57.19324	N/A	41.7	27.09%	N/A
2 ethanol	-47174.5	-47174.5	N/A	N/A	44.1	N/A	N/A
3 ethanol	0.656067	0.656375	24.82339	N/A	44.1	77.66%	N/A
4 ethanol	0.44137	0.441139	32.18146	N/A	48.3	50.09%	N/A
5 ethanol	N/A	N/A	N/A	N/A	47.6	N/A	N/A
6	18.50902	18.50965	2.65E-12	2.65015E-12	6.00E-7	22616128.82%	22640162.91%
7	18.38455	18.38477	3.27E-12	3.27239E-12	1.10E-6	33601626.50%	33614518.39%
8	17.77618	17.77609	9.15E-12	9.14811E-12	1.00E-6	10932828.48%	10931124.11%
9	15.4279	15.42858	4.83E-10	4.82192E-10	4.00E-5	8285907.99%	8295354.77%
10	13.43476	13.43435	1.4E-8	1.3995E-8	5.50E-4	3932589.09%	3929868.82%
11	10.25339	10.25351	3.01E-6	3.01375E-6	1.40E-2	464346.84%	464437.46%
12	36.06504	36.06548	3.52E-25	3.51688E-25	0	0%	0%
13 CDCl3	-2.06205	-2.06137	97.01905	97.01572446	86	11.36%	11.35%
13 DMSO	-2.06205	-2.06137	97.01905	97.01572446	63	35.06%	35.06%
13	-2.06205	-2.06137	97.01905	97.01572446	80	17.54%	17.54%
14 CDCl3	1.423478	1.423819	8.285603	8.281221474	3	63.79%	63.77%
14 DMSO	1.423478	1.423819	8.285603	8.281221474	0	0%	0%

14	1.423478	1.423819	8.285603	8.281221474	8	3.45%	3.40%
15 CDCl3	-0.47035	-0.47063	68.87739	68.88753447	85	23.41%	23.39%
15 DMSO	-0.47035	-0.47063	68.87739	68.88753447	99	43.73%	43.71%
15	-0.47035	-0.47063	68.87739	68.88753447	89	29.22%	29.20%
16	0.391978	0.392193	34.02848	34.02031827	80	135.10%	135.15%
17	N/A	N/A	N/A	N/A	91.7	N/A	N/A
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	N/A	N/A	N/A	N/A	95.8	N/A	N/A
20	9.006888	9.006644	2.47E-5	2.47556E-5	95.3	385121692.57%	384963239.30%
21	-1.39944	-1.39935	91.40056	91.39937366	98	7.22%	7.22%
22	-0.9342	-0.93499	82.88926	82.90819974	82.1	0.95%	0.97%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-2.34403	-2.34438	98.12734	98.1284234	93.4	4.82%	4.82%
25	9.894947	9.89457	5.52E-6	5.52567E-6	91.6	1658775183.82%	1657718908.43%
26	-1.97478	-1.97477	96.5619	96.56188449	93.7	2.96%	2.96%
27	N/A	N/A	N/A	N/A	85.2	N/A	N/A
28	N/A	N/A	N/A	N/A	88.5	N/A	N/A
29	-1.41116	-1.41064	91.55497	91.54815529	89.2	2.57%	2.56%
30	-1.05991	-1.05986	85.69418	85.69321515	90.8	5.96%	5.96%
31	-1.67477	-1.67482	94.42004	94.42053432	93.4	1.08%	1.08%

32	-0.5834	-0.58296	72.81618	72.80150249	93.7	28.68%	28.71%
33	-3.14785	-3.14822	99.51141	99.51171343	94.6	4.94%	4.94%
34	-1.13834	-1.13767	87.24257	87.23009003	93.9	7.63%	7.65%
35	-0.93944	-0.93938	83.01457	83.01307074	95.9	15.52%	15.52%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	N/A	N/A	N/A	N/A	40.5	N/A	N/A
42 CDCl3	-2.42747	-2.42783	98.36948	98.37047516	92.6	5.87%	5.87%
43 DMSO	-2.1686	-2.16867	97.4977	97.49801026	94	3.59%	3.59%
43 Acetone	-2.1686	-2.16867	97.4977	97.49801026	97.7	0.21%	0.21%
43 CDCl3	-2.1686	-2.16867	97.4977	97.49801026	97.8	0.31%	0.31%
44 DMSO	-4.04663	-4.04681	99.89251	99.89254666	90.2	9.70%	9.70%
44 Acetone	-4.04663	-4.04681	99.89251	99.89254666	93.6	6.30%	6.30%
44 CDCl3	-4.04663	-4.04681	99.89251	99.89254666	91.6	8.30%	8.30%
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A
45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A

46 DMSO	13.69758	13.6979	8.97E-9	8.96723E-9	93.7	1044339816980.44 %	1044916256051.01 %
46 Acetone	13.69758	13.6979	8.97E-9	8.96723E-9	97.3	1084463865448.84 %	1085062451591.50 %
46 CDCl3	13.69758	13.6979	8.97E-9	8.96723E-9	95.7	1066630955018.44 %	1067219698017.95 %
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A

51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	-1.82483	-1.8248	95.61451	95.61425778	95	0.64%	0.64%
52 Acetone	-1.82483	-1.8248	95.61451	95.61425778	96.7	1.14%	1.14%
52 CDCl3	-1.82483	-1.8248	95.61451	95.61425778	97.9	2.39%	2.39%
Mean Error of Theoretical Calculation of Gas Phase vs literature						6.95E8%	7.44E8%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						18.24%	15.11%

Table 1.17: Convergence results from M05 631++G gas phase and how it compares to experimental data.

1.4.3 M05 6-31+G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.17442	-0.17445	57.31162	57.31293964	41.7	27.24%	27.24%
2 ethanol	-47174.4	-47174.4	N/A	N/A	44.1	N/A	N/A
3 ethanol	-0.19342	-0.19327	58.09502	58.08893317	44.1	24.09%	24.08%
4 ethanol	N/A	N/A	N/A	N/A	48.3	N/A	N/A
5 ethanol	0.034886	0.035141	48.52744	48.51668424	47.6	1.91%	1.89%
6	18.64017	18.6408	2.13E-12	2.1236E-12	6.00E-7	28224157.38%	28253834.26%
7	18.41799	18.41866	3.09E-12	3.09036E-12	1.10E-6	35554114.00%	35594411.14%
8	17.87685	17.87649	7.72E-12	7.72124E-12	1.00E-6	12959116.14%	12951182.91%
9	15.5123	15.51266	4.19E-10	4.18353E-10	4.00E-5	9555402.84%	9561202.16%
10	13.485	13.48455	1.28E-08	1.28574E-08	5.50E-4	4280871.10%	4277607.66%
11	10.34378	10.34324	2.59E-06	2.58993E-06	1.40E-2	540950.75%	540455.21%
12	35.74809	35.74796	6.01E-25	6.01252E-25	0	0%	0%
13 CDCl3	-0.32021	-0.32003	63.20024	63.19308958	86	36.08%	36.09%
13 DMSO	-0.32021	-0.32003	63.20024	63.19308958	63	0.32%	0.31%
13	-0.32021	-0.32003	63.20024	63.19308958	80	26.58%	26.60%
14 CDCl3	1.547918	1.548066	6.822177	6.820585746	3	56.03%	56.02%
14 DMSO	1.547918	1.548066	6.822177	6.820585746	0	0%	0%

14	1.547918	1.548066	6.822177	6.820585746	8	17.26%	17.29%
15 CDCl3	-0.46761	-0.46687	68.77802	68.7510825	85	23.59%	23.63%
15 DMSO	-0.46761	-0.46687	68.77802	68.7510825	99	43.94%	44.00%
15	-0.46761	-0.46687	68.77802	68.7510825	89	29.40%	29.45%
16	0.05096	0.050828	47.84964	47.85517699	80	67.19%	67.17%
17	-1.1128	-1.1132	86.75467	86.76254437	91.7	5.70%	5.69%
18	-1.25659	-1.25753	89.30519	89.32029739	91.7	2.68%	2.66%
19	N/A	N/A	N/A	N/A	95.8	N/A	N/A
20	9.068761	9.069395	2.23E-05	2.22662E-05	95.3	427545230.60%	428002943.36%
21	-1.4808	-1.48029	92.42095	92.41502785	98	6.04%	6.04%
22	-0.89171	-0.89169	81.84748	81.84687502	82.1	0.31%	0.31%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-2.25169	-2.25213	97.81818	97.81978214	93.4	4.52%	4.52%
25	9.960707	9.960458	4.94E-06	4.94374E-06	91.6	1853627212.87%	1852847864.14%
26	-1.9385	-1.939	96.35261	96.35558929	93.7	2.75%	2.76%
27	N/A	N/A	N/A	N/A	85.2	N/A	N/A
28	N/A	N/A	N/A	N/A	88.5	N/A	N/A
29	-1.41222	-1.41252	91.56876	91.57272396	89.2	2.59%	2.59%
30	-0.68509	-0.68524	76.07991	76.08464748	90.8	19.35%	19.34%
31	N/A	N/A	N/A	N/A	93.4	N/A	N/A

32	-0.54178	-0.54154	71.40268	71.3945973	93.7	31.23%	31.24%
33	-3.17919	-3.17959	99.53648	99.53679793	94.6	4.96%	4.96%
34	N/A	N/A	N/A	N/A	93.9	N/A	N/A
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	0.208394	0.208333	41.29065	41.29312103	40.5	1.91%	1.92%
42 CDCl3	-2.39976	-2.40022	98.2927	98.2940143	92.6	5.79%	5.79%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A
45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A

46 DMSO	-2.48115	-2.4818	98.50871	98.51031556	93.7	4.88%	4.88%
46 Acetone	-2.48115	-2.4818	98.50871	98.51031556	97.3	1.23%	1.23%
46 CDCl3	-2.48115	-2.4818	98.50871	98.51031556	95.7	2.85%	2.85%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	13.25561	13.25551	1.89E-08	1.89301E-08	90.7	479215486445.62 %	479132181441.58 %
48 Acetone	13.25561	13.25551	1.89E-08	1.89301E-08	95.3	503519689732.39 %	503432159777.76 %
48 CDCl3	13.25561	13.25551	1.89E-08	1.89301E-08	95.2	502991337487.02 %	502903899379.15 %
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-1.69816	-1.69867	94.62462	94.62894374	94.6	0.03%	0.03%
50 Acetone	-1.69816	-1.69867	94.62462	94.62894374	97.8	3.36%	3.35%
50 CDCl3	-1.69816	-1.69867	94.62462	94.62894374	97.2	2.72%	2.72%
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A

51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						3.46E8%	3.46E8%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.27%	14.27%

Table 1.18: Convergence results from M05 631+G gas phase and how it compares to experimental data.

1.4.4 M05 6-31G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-1.44133	-0.26481	91.9407	60.99840052	41.7	54.64%	31.64%
2 ethanol	-47172.3	-47172.5	N/A	N/A	44.1	N/A	N/A
3 ethanol	0.831786	-0.34262	19.70505	64.07596915	44.1	123.80%	31.18%
4 ethanol	-1.33546	0.626254	90.51237	25.77487364	48.3	46.64%	87.39%
5 ethanol	-1.53305	-0.1801	93.01649	57.54613417	47.6	48.83%	17.28%
6	20.05262	19.15033	1.96E-13	8.98109E-13	6.00E-7	306647858.21%	66806933.87%
7	18.75986	19.68874	1.74E-12	3.61754E-13	1.10E-6	63336501.31%	304074071.77%
8	18.68791	18.3534	1.96E-12	3.45047E-12	1.00E-6	50989592.04%	28981459.60%
9	16.45194	16.0404	8.56E-11	1.71574E-10	4.00E-5	46716967.76%	23313442.86%
10	14.13678	14.62599	4.27E-09	1.8703E-09	5.50E-4	12871039.52%	29406934.84%
11	12.89804	11.95845	3.46E-08	1.69255E-07	1.40E-2	40436327.07%	8271466.55%
12	37.59251	35.81699	2.67E-26	5.35089E-25	0	0.00%	0.00%
13 CDCl3	-3.08537	-2.27849	99.45733	97.91271973	86	13.53%	12.17%
13 DMSO	-3.08537	-2.27849	99.45733	97.91271973	63	36.66%	35.66%
13	-3.08537	-2.27849	99.45733	97.91271973	80	19.56%	18.29%
14 CDCl3	N/A	N/A	N/A	N/A	3	N/A	N/A
14 DMSO	N/A	N/A	N/A	N/A	0	N/A	N/A

14	N/A	N/A	N/A	N/A	8	N/A	N/A
15 CDCl3	N/A	N/A	N/A	N/A	85	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99	N/A	N/A
15	N/A	N/A	N/A	N/A	89	N/A	N/A
16	-1.72877	-0.26481	94.88158	60.99840052	80	15.68%	31.15%
17	-3.28921	-2.52635	99.61478	98.61680322	91.7	7.95%	7.01%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-4.77623	-2.74786	99.96863	99.04437869	95.8	4.17%	3.28%
20	6.854895	8.796428	0.000937	3.53074E-05	95.3	10165346.19%	269915080.22%
21	-4.45495	-1.70745	99.94604	94.70385904	98	1.95%	3.48%
22	-2.75188	-1.63466	99.05078	94.05224694	82.1	17.11%	12.71%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-4.03063	-3.37663	99.88957	99.6674829	93.4	6.50%	6.29%
25	9.482643	10.03576	1.11E-05	4.35334E-06	91.6	826731536.89%	2104130906.30%
26	-3.58883	-2.20193	99.7674	97.63143732	93.7	6.08%	4.03%
27	N/A	N/A	N/A	N/A	85.2	N/A	N/A
28	-2.35027	0.109814	98.14662	45.37652358	88.5	9.83%	95.03%
29	-5.72143	-3.47138	99.99364	99.71651762	89.2	10.79%	10.55%
30	-3.69742	-2.63554	99.8063	98.84705408	90.8	9.02%	8.14%
31	-4.01025	-1.7746	99.88571	95.24464434	93.4	6.49%	1.94%

32	-4.1317	-2.7121	99.90689	98.98547412	93.7	6.21%	5.34%
33	-2.04691	-0.7869	96.94419	79.06780032	94.6	2.42%	19.64%
34	-3.64285	-1.50226	99.78764	92.67098598	93.9	5.90%	1.33%
35	-3.69966	-1.51293	99.80703	92.79241809	95.9	3.91%	3.35%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-1.48556	-0.20018	92.47709	58.37248572	40.5	56.21%	30.62%
42 CDCl3	N/A	N/A	N/A	N/A	92.6	N/A	N/A
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-6.51877	-3.63705	99.99835	99.78555592	90.2	9.80%	9.61%
44 Acetone	-6.51877	-3.63705	99.99835	99.78555592	93.6	6.40%	6.20%
44 CDCl3	-6.51877	-3.63705	99.99835	99.78555592	91.6	8.40%	8.20%
45 DMSO	-1.80964	-1.37425	95.50565	91.06022521	94.6	0.95%	3.89%
45Acetone	-1.80964	-1.37425	95.50565	91.06022521	99.3	3.97%	9.05%
45 CDCl3	-1.80964	-1.37425	95.50565	91.06022521	97.3	1.88%	6.85%

46 DMSO	-4.68763	-2.25903	99.96357	97.84450695	93.7	6.27%	4.24%
46 Acetone	-4.68763	-2.25903	99.96357	97.84450695	97.3	2.66%	0.56%
46 CDCl3	-4.68763	-2.25903	99.96357	97.84450695	95.7	4.27%	2.19%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	-4.03133	-2.61232	99.8897	98.8014976	90.7	9.20%	8.20%
48 Acetone	-4.03133	-2.61232	99.8897	98.8014976	95.3	4.59%	3.54%
48 CDCl3	-4.03133	-2.61232	99.8897	98.8014976	95.2	4.69%	3.65%
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-4.50839	-1.99234	99.95069	96.65905313	94.6	5.35%	2.13%
50 Acetone	-4.50839	-1.99234	99.95069	96.65905313	97.8	2.15%	1.18%
50 CDCl3	-4.50839	-1.99234	99.95069	96.65905313	97.2	2.75%	0.56%
51 DMSO	-3.90965	-2.34877	99.86457	98.14199977	94	5.87%	4.22%
51 Acetone	-3.90965	-2.34877	99.86457	98.14199977	96.4	3.47%	1.77%
51 CDCl3	-3.90965	-2.34877	99.86457	98.14199977	96.1	3.77%	2.08%
52 DMSO	-3.80859	-2.19942	99.83941	97.62161431	95	4.85%	2.69%
52 Acetone	-3.80859	-2.19942	99.83941	97.62161431	96.7	3.14%	0.94%

52 CDCl3	-3.80859	-2.19942	99.83941	97.62161431	97.9	1.94%	0.29%
Mean Error of Theoretical Calculation of Gas Phase vs literature						2.56E5%	5.35E5%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						13.56%	12.43%

Table 1.19: Convergence results from M05 6-31G gas phase and how it compares to experimental data.

1.4.5 M05 cc-pVDZ

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.25009	-0.25038	60.4054	60.41695897	41.7	30.97%	30.98%
2 ethanol	-47174.3	-47174.3	N/A	N/A	44.1	N/A	N/A
3 ethanol	0.333836	0.333835	36.26625	36.26627915	44.1	21.60%	21.60%
4 ethanol	0.664072	0.663905	24.57196	24.57717225	48.3	96.57%	96.52%
5 ethanol	-1.30052	-1.30083	89.99345	89.99808217	47.6	47.11%	47.11%
6	19.72037	19.72011	3.43E-13	3.43083E-13	6.00E-7	174960711.34%	174884611.63%
7	19.46177	19.46158	5.31E-13	5.30924E-13	1.10E-6	207252165.55%	207185706.57%
8	17.8894	17.88904	7.55E-12	7.5593E-12	1.00E-6	13236722.44%	13228634.16%
9	15.87456	15.87411	2.27E-10	2.27209E-10	4.00E-5	17618365.81%	17604875.07%
10	14.48278	14.48355	2.38E-09	2.379E-09	5.50E-4	23089037.92%	23118888.15%
11	12.21558	12.21573	1.1E-07	1.09604E-07	1.40E-2	12770001.00%	12773123.10%
12	36.2572	36.2575	2.54E-25	2.54281E-25	0	0%	0%
13 CDCl3	-2.11936	-2.1191	97.28661	97.28544064	86	11.60%	11.60%
13 DMSO	-2.11936	-2.1191	97.28661	97.28544064	63	35.24%	35.24%
13	-2.11936	-2.1191	97.28661	97.28544064	80	17.77%	17.77%
14 CDCl3	0.506231	0.505773	29.83868	29.8549052	3	89.95%	89.95%
14 DMSO	0.506231	0.505773	29.83868	29.8549052	0	0%	0%

14	0.506231	0.505773	29.83868	29.8549052	8	73.19%	73.20%
15 CDCl3	-1.5081	-1.50791	92.73775	92.73550646	85	8.34%	8.34%
15 DMSO	-1.5081	-1.50791	92.73775	92.73550646	99	6.75%	6.76%
15	-1.5081	-1.50791	92.73775	92.73550646	89	4.03%	4.03%
16	-0.03142	-0.03138	51.32626	51.32446788	80	55.87%	55.87%
17	-1.33292	-1.33283	90.47559	90.47421394	91.7	1.35%	1.35%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	N/A	N/A	N/A	N/A	95.8	N/A	N/A
20	8.969655	8.969621	2.64E-05	2.6353E-05	95.3	361649874.77%	361628822.83%
21	-2.01862	-2.0187	96.79946	96.79985119	98	1.24%	1.24%
22	-1.33307	-1.33283	90.47765	90.47421394	82.1	9.26%	9.26%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-3.2363	-3.23607	99.57893	99.57876078	93.4	6.21%	6.20%
25	10.18598	10.18636	3.38E-06	3.37564E-06	91.6	2711794178.52%	2713555721.46%
26	-2.49751	-2.49749	98.54875	98.54870197	93.7	4.92%	4.92%
27	-3.86828	-3.8686	99.85479	99.85486433	85.2	14.68%	14.68%
28	N/A	N/A	N/A	N/A	88.5	N/A	N/A
29	-3.91157	-3.91127	99.86501	99.86494232	89.2	10.68%	10.68%
30	-2.75373	-2.75351	99.05371	99.05336458	90.8	8.33%	8.33%
31	-1.79923	-1.79907	95.4296	95.4283886	93.4	2.13%	2.13%

32	N/A	N/A	N/A	N/A	93.7	N/A	N/A
33	N/A	N/A	N/A	N/A	94.6	N/A	N/A
34	N/A	N/A	N/A	N/A	93.9	N/A	N/A
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	0.185048	0.185115	42.24963	42.24686312	40.5	4.14%	4.13%
42 CDCl3	-3.83371	-3.83346	99.84607	99.84600344	92.6	7.26%	7.26%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-3.42644	-3.4262	99.69423	99.6941079	90.2	9.52%	9.52%
44 Acetone	-3.42644	-3.4262	99.69423	99.6941079	93.6	6.11%	6.11%
44 CDCl3	-3.42644	-3.4262	99.69423	99.6941079	91.6	8.12%	8.12%
45 DMSO	-1.54617	-1.54618	93.15899	93.15917977	94.6	1.55%	1.55%
45Acetone	-1.54617	-1.54618	93.15899	93.15917977	99.3	6.59%	6.59%
45 CDCl3	-1.54617	-1.54618	93.15899	93.15917977	97.3	4.45%	4.44%

46 DMSO	N/A	N/A	N/A	N/A	93.7	N/A	N/A
46 Acetone	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 CDCl3	N/A	N/A	N/A	N/A	95.7	N/A	N/A
47 DMSO	-3.44188	-3.44189	99.70208	99.70208242	70.1	29.69%	29.69%
47 Acetone	-3.44188	-3.44189	99.70208	99.70208242	87.1	12.64%	12.64%
47 CDCl3	-3.44188	-3.44189	99.70208	99.70208242	86.6	13.14%	13.14%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A

52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						8.19E5%	8.20E5%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						18.89%	18.88%

Table 1.20: Convergence results from M05 cc-pVDZ gas phase and how it compares to experimental data.

1.5 M05-2X gas phase

1.5.1 M05-2X 6311++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-2.805	-2.72151	99.13152	99.00131505	41.7	57.93%	57.88%
2 ethanol	-47200.9	-47200.9	N/A	N/A	44.1	N/A	N/A
3 ethanol	-2.50672	-2.5069	98.57083	98.57126429	44.1	55.26%	55.26%
4 ethanol	-2.30076	-2.30108	97.98823	97.98928578	48.3	50.71%	50.71%
5 ethanol	-2.73327	-2.7328	99.02076	99.02000126	47.6	51.93%	51.93%
6	13.73859	13.73807	8.37E-09	8.37916E-09	6.00E-7	7066.92%	7060.62%
7	13.34934	13.34964	1.62E-08	1.61477E-08	1.10E-6	6708.74%	6712.12%
8	13.2203	13.22037	2.01E-08	2.00876E-08	1.00E-6	4877.61%	4878.20%
9	10.78343	10.78312	1.23E-06	1.23207E-06	4.00E-5	3148.25%	3146.57%
10	8.695942	8.695399	4.18E-05	4.18764E-05	5.50E-4	1214.59%	1213.39%
11	6.116775	6.116335	0.003261	0.003263517	1.40E-2	329.30%	328.99%
12	29.44444	29.44463	2.53E-20	2.5265E-20	0	0%	0%
13 CDCl3	N/A	N/A	N/A	N/A	86	N/A	N/A
13 DMSO	N/A	N/A	N/A	N/A	63	N/A	N/A
13	N/A	N/A	N/A	N/A	80	N/A	N/A
14 CDCl3	-2.65174	-2.65123	98.87783	98.87686229	3	96.97%	96.97%

14 DMSO	-2.65174	-2.65123	98.87783	98.87686229	0	0%	0%
14	-2.65174	-2.65123	98.87783	98.87686229	8	91.91%	91.91%
15 CDCl3	N/A	N/A	N/A	N/A	85	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99	N/A	N/A
15	N/A	N/A	N/A	N/A	89	N/A	N/A
16	-3.29682	-3.29693	99.61968	99.6197573	80	19.69%	19.69%
17	-4.89434	-4.89457	99.9743	99.9743112	91.7	8.28%	8.28%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-5.32101	-5.32003	99.9875	99.98747624	95.8	4.19%	4.19%
20	6.127427	6.127003	0.003203	0.003205247	95.3	2975281.24%	2973150.07%
21	-4.78235	-4.78225	99.96895	99.96894656	98	1.97%	1.97%
22	-2.34494	-2.34438	98.13017	98.1284234	82.1	16.34%	16.33%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-5.55907	-5.55911	99.99164	99.9916365	93.4	6.59%	6.59%
25	6.559365	6.558729	0.001544	0.001545964	91.6	5931373.09%	5925003.90%
26	-5.37869	-5.37838	99.98866	99.98865161	93.7	6.29%	6.29%
27	-4.34009	-4.33986	99.93449	99.93446795	85.2	14.74%	14.74%
28	-4.11057	-4.11081	99.90351	99.90354612	88.5	11.41%	11.41%
29	-4.87801	-4.87889	99.97358	99.97362165	89.2	10.78%	10.78%
30	-3.84276	-3.84224	99.8484	99.84826806	90.8	9.06%	9.06%

31	-5.40021	-5.40035	99.98906	99.98906481	93.4	6.59%	6.59%
32	-4.16465	-4.16415	99.91192	99.91184795	93.7	6.22%	6.22%
33	N/A	N/A	N/A	N/A	94.6	N/A	N/A
34	-4.43203	-4.4321	99.94391	99.94391659	93.9	6.05%	6.05%
35	-4.25519	-4.25514	99.9244	99.9243956	95.9	4.03%	4.03%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-2.60938	-2.60918	98.7956	98.79520646	40.5	59.01%	59.01%
42 CDCl3	-5.04175	-5.04141	99.97996	99.97995233	92.6	7.38%	7.38%
43 DMSO	-5.3221	-5.32191	99.98752	99.987516	94	5.99%	5.99%
43 Acetone	-5.3221	-5.32191	99.98752	99.987516	97.7	2.29%	2.29%
43 CDCl3	-5.3221	-5.32191	99.98752	99.987516	97.8	2.19%	2.19%
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A

45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 DMSO	-5.11143	-5.11169	99.98219	99.98219578	93.7	6.28%	6.28%
46 Acetone	-5.11143	-5.11169	99.98219	99.98219578	97.3	2.68%	2.68%
46 CDCl3	-5.11143	-5.11169	99.98219	99.98219578	95.7	4.28%	4.28%
47 DMSO	-6.95663	-6.95657	99.99921	99.99921043	70.1	29.90%	29.90%
47 Acetone	-6.95663	-6.95657	99.99921	99.99921043	87.1	12.90%	12.90%
47 CDCl3	-6.95663	-6.95657	99.99921	99.99921043	86.6	13.40%	13.40%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-4.98392	-4.98368	99.97791	99.97789959	94.6	5.38%	5.38%
50 Acetone	-4.98392	-4.98368	99.97791	99.97789959	97.8	2.18%	2.18%
50 CDCl3	-4.98392	-4.98368	99.97791	99.97789959	97.2	2.78%	2.78%
51 DMSO	-4.36784	-4.36747	99.93749	99.93745183	94	5.94%	5.94%
51 Acetone	-4.36784	-4.36747	99.93749	99.93745183	96.4	3.54%	3.54%
51 CDCl3	-4.36784	-4.36747	99.93749	99.93745183	96.1	3.84%	3.84%
52 DMSO	-5.08179	-5.08157	99.98127	99.98126679	95	4.98%	4.98%

52 Acetone	-5.08179	-5.08157	99.98127	99.98126679	96.7	3.28%	3.28%
52 CDCl3	-5.08179	-5.08157	99.98127	99.98126679	97.9	2.08%	2.08%
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.79E3%	1.75E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						15.70%	16.68%

Table 1.21: Convergence results from M05-2X 6-311++G gas phase and how it compares to experimental data.

1.5.2 M05-2X 6-31++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-2.76534	-2.76543	99.07192	99.07206087	41.7	57.91%	57.91%
2 ethanol	-47187.3	-47187.3	N/A	N/A	44.1	N/A	N/A
3 ethanol	-2.14453	-2.1442	97.3966	97.39517859	44.1	54.72%	54.72%
4 ethanol	-2.53032	-2.53012	98.62591	98.62545045	48.3	51.03%	51.03%
5 ethanol	-2.7608	-2.76104	99.06483	99.06521571	47.6	51.95%	51.95%
6	14.31863	14.31851	3.14E-09	3.14374E-09	6.00E-7	18989.29%	18985.57%
7	13.63004	13.63013	1.01E-08	1.00547E-08	1.10E-6	10838.50%	10840.19%
8	13.41887	13.41866	1.44E-08	1.43708E-08	1.00E-6	6860.99%	6858.56%
9	10.9171	10.91678	9.83E-07	9.83098E-07	4.00E-5	3970.95%	3968.77%
10	8.787382	8.787016	3.59E-05	3.58732E-05	5.50E-4	1434.13%	1433.18%
11	N/A	N/A	N/A	N/A	1.40E-2	N/A	N/A
12	N/A	N/A	N/A	N/A	0	N/A	N/A
13 CDCl3	-4.91844	-4.91779	99.97533	99.97529881	86	13.98%	13.98%
13 DMSO	-4.91844	-4.91779	99.97533	99.97529881	63	36.98%	36.98%
13	-4.91844	-4.91779	99.97533	99.97529881	80	19.98%	19.98%
14 CDCl3	N/A	N/A	N/A	N/A	3	N/A	N/A
14 DMSO	N/A	N/A	N/A	N/A	0	N/A	N/A

14	N/A	N/A	N/A	N/A	8	N/A	N/A
15 CDCl3	N/A	N/A	N/A	N/A	85	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99	N/A	N/A
15	N/A	N/A	N/A	N/A	89	N/A	N/A
16	-4.46583	-4.46599	99.94702	99.9470345	80	19.96%	19.96%
17	-6.77473	-6.77459	99.99893	99.99892634	91.7	8.30%	8.30%
18	-5.35167	-5.3514	99.98813	99.98812254	91.7	8.29%	8.29%
19	-6.44768	-6.44766	99.99814	99.99813505	95.8	4.20%	4.20%
20	5.959445	5.95883	0.004254	0.004258048	95.3	2240339.77%	2238014.62%
21	-5.98285	-5.98268	99.99591	99.99591002	98	2.00%	2.00%
22	-4.81135	-4.81174	99.97044	99.97045504	82.1	17.88%	17.88%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	N/A	N/A	N/A	N/A	93.4	N/A	N/A
25	6.407144	6.406872	0.001997	0.001997948	91.6	4586713.38%	4584604.99%
26	-6.49124	-6.49159	99.99827	99.9982684	93.7	6.30%	6.30%
27	-5.63412	-5.63441	99.99263	99.99263523	85.2	14.79%	14.79%
28	N/A	N/A	N/A	N/A	88.5	N/A	N/A
29	-5.94669	-5.94628	99.99565	99.99565074	89.2	10.80%	10.80%
30	-5.23241	-5.23217	99.98548	99.98547339	90.8	9.19%	9.19%
31	-6.51436	-6.5148	99.99833	99.99833498	93.4	6.60%	6.60%

32	-4.87096	-4.87073	99.97327	99.9732558	93.7	6.27%	6.27%
33	-9.13442	-9.13466	99.99998	99.99998006	94.6	5.40%	5.40%
34	-5.45017	-5.45055	99.98995	99.98995365	93.9	6.09%	6.09%
35	-5.09615	-5.09538	99.98172	99.98169845	95.9	4.08%	4.08%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-3.84262	-3.84224	99.84836	99.84826806	40.5	59.44%	59.44%
42 CDCl3	-6.42753	-6.42758	99.99807	99.99807072	92.6	7.40%	7.40%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A
45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A

46 DMSO	N/A	N/A	N/A	N/A	93.7	N/A	N/A
46 Acetone	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 CDCl3	N/A	N/A	N/A	N/A	95.7	N/A	N/A
47 DMSO	-7.85485	-7.85454	99.99983	99.99982672	70.1	29.90%	29.90%
47 Acetone	-7.85485	-7.85454	99.99983	99.99982672	87.1	12.90%	12.90%
47 CDCl3	-7.85485	-7.85454	99.99983	99.99982672	86.6	13.40%	13.40%
48 DMSO	9.273163	9.273335	1.58E-05	1.57782E-05	90.7	574677049.24%	574844656.52%
48 Acetone	9.273163	9.273335	1.58E-05	1.57782E-05	95.3	603822748.10%	603998855.86%
48 CDCl3	9.273163	9.273335	1.58E-05	1.57782E-05	95.2	603189145.95%	603365068.92%
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	-6.00413	-6.00401	99.99606	99.99605477	95	5.00%	5.00%
52 Acetone	-6.00413	-6.00401	99.99606	99.99605477	96.7	3.30%	3.30%

52 CDCl3	-6.00413	-6.00401	99.99606	99.99605477	97.9	2.10%	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						4.47E5%	4.47E5%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						18.34%	18.34%

Table 1.22: Convergence results M05-2X 6-31++G gas phase and how it compares to experimental data.

1.5.3 M05-2X 6-31+G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-2.79943	-2.79995	99.12339	99.12414418	41.7	57.93%	57.93%
2 ethanol	-47187.5	-47187.5	N/A	N/A	44.1	N/A	N/A
3 ethanol	-1.45493	-1.45519	92.10918	92.11247345	44.1	52.12%	52.12%
4 ethanol	-2.50844	-2.50878	98.57493	98.5757351	48.3	51.00%	51.00%
5 ethanol	-2.74951	-2.74975	99.04701	99.04738334	47.6	51.94%	51.94%
6	14.41398	14.41389	2.68E-09	2.67599E-09	6.00E-7	22324.80%	22321.61%
7	13.6729	13.6728	9.35E-09	9.35555E-09	1.10E-6	11659.57%	11657.73%
8	13.53222	13.53224	1.19E-08	1.18623E-08	1.00E-6	8329.71%	8330.03%
9	10.99555	10.99522	8.61E-07	8.61117E-07	4.00E-5	4547.72%	4545.13%
10	8.943586	8.942638	2.75E-05	2.75817E-05	5.50E-4	1897.27%	1894.07%
11	6.071028	6.071154	0.003523	0.003522286	1.40E-2	297.38%	297.47%
12	N/A	N/A	N/A	N/A	0	N/A	N/A
13 CDCl3	-6.07138	-6.07178	99.99648	99.99648145	86	14.00%	14.00%
13 DMSO	-6.07138	-6.07178	99.99648	99.99648145	63	37.00%	37.00%
13	-6.07138	-6.07178	99.99648	99.99648145	80	20.00%	20.00%
14 CDCl3	N/A	N/A	N/A	N/A	3	N/A	N/A
14 DMSO	N/A	N/A	N/A	N/A	0	N/A	N/A

14	N/A	N/A	N/A	N/A	8	N/A	N/A
15 CDCl3	-4.98228	-4.98243	99.97785	99.9778527	85	14.98%	14.98%
15 DMSO	-4.98228	-4.98243	99.97785	99.9778527	99	0.98%	0.98%
15	-4.98228	-4.98243	99.97785	99.9778527	89	10.98%	10.98%
16	-4.44263	-4.44277	99.9449	99.94491745	80	19.96%	19.96%
17	N/A	N/A	N/A	N/A	91.7	N/A	N/A
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-6.44855	-6.44829	99.99814	99.99813703	95.8	4.20%	4.20%
20	6.000823	6.000873	0.003967	0.003966189	95.3	2402505.19%	2402710.26%
21	-5.94826	-5.94816	99.99567	99.99566454	98	2.00%	2.00%
22	-4.76801	-4.76844	99.96819	99.96821424	82.1	17.87%	17.87%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-6.76141	-6.76141	99.9989	99.99890218	93.4	6.60%	6.60%
25	6.464071	6.463975	0.001814	0.001814261	91.6	5049601.86%	5048786.62%
26	-6.44927	-6.44954	99.99814	99.99814097	93.7	6.30%	6.30%
27	-5.60607	-5.60617	99.99227	99.99227551	85.2	14.79%	14.79%
28	-5.06655	-5.06651	99.98079	99.98078428	88.5	11.48%	11.48%
29	-5.91412	-5.91365	99.99541	99.99540433	89.2	10.80%	10.80%
30	-5.27736	-5.27735	99.98654	99.98654049	90.8	9.19%	9.19%
31	-6.47583	-6.4759	99.99822	99.99822191	93.4	6.60%	6.60%

32	-4.8248	-4.82429	99.9711	99.97107452	93.7	6.27%	6.27%
33	-10.9609	-10.9613	100	99.99999909	94.6	5.40%	5.40%
34	-5.51261	-5.51267	99.99095	99.99095424	93.9	6.09%	6.09%
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-3.90407	-3.90374	99.86329	99.86321607	40.5	59.44%	59.44%
42 CDCl3	-6.39191	-6.39244	99.99795	99.99795275	92.6	7.40%	7.40%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-6.8623	-6.86244	99.99907	99.99907439	94.6	5.40%	5.40%
45Acetone	-6.8623	-6.86244	99.99907	99.99907439	99.3	0.70%	0.70%
45 CDCl3	-6.8623	-6.86244	99.99907	99.99907439	97.3	2.70%	2.70%

46 DMSO	-6.17055	-6.1703	99.99702	99.99702077	93.7	6.30%	6.30%
46 Acetone	-6.17055	-6.1703	99.99702	99.99702077	97.3	2.70%	2.70%
46 CDCl3	-6.17055	-6.1703	99.99702	99.99702077	95.7	4.30%	4.30%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	-7.89623	-7.89595	99.99984	99.99983843	82.5	17.50%	17.50%
49 Acetone	-7.89623	-7.89595	99.99984	99.99983843	92	8.00%	8.00%
49 CDCl3	-7.89623	-7.89595	99.99984	99.99983843	88.2	11.80%	11.80%
50 DMSO	-6.05143	-6.0517	99.99636	99.99636007	94.6	5.40%	5.40%
50 Acetone	-6.05143	-6.0517	99.99636	99.99636007	97.8	2.20%	2.20%
50 CDCl3	-6.05143	-6.0517	99.99636	99.99636007	97.2	2.80%	2.80%
51 DMSO	-6.05687	-6.05672	99.99639	99.9963908	94	6.00%	6.00%
51 Acetone	-6.05687	-6.05672	99.99639	99.9963908	96.4	3.60%	3.60%
51 CDCl3	-6.05687	-6.05672	99.99639	99.9963908	96.1	3.90%	3.90%
52 DMSO	-5.87602	-5.876	99.9951	99.99510262	95	5.00%	5.00%
52 Acetone	-5.87602	-5.876	99.9951	99.99510262	96.7	3.30%	3.30%

52 CDCl3	-5.87602	-5.876	99.9951	99.99510262	97.9	2.10%	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.44E3%	1.44E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						13.61%	13.61%

Table 1.23: Convergence results M05-2X 6-31+G gas phase and how it compares to experimental data.

1.5.4 M05-2X 6-31G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-2.77277	-2.77296	99.08338	99.08368009	41.7	57.91%	57.91%
2 ethanol	-47185.9	-47185.9	N/A	N/A	44.1	N/A	N/A
3 ethanol	-2.57882	-2.22076	98.73261	97.70385841	44.1	55.33%	54.86%
4 ethanol	N/A	N/A	N/A	N/A	48.3	N/A	N/A
5 ethanol	-2.81354	-2.81375	99.14386	99.14415672	47.6	51.99%	51.99%
6	15.17394	15.17318	7.41E-10	7.42253E-10	6.00E-7	80839.06%	80735.02%
7	14.97255	14.97238	1.04E-09	1.04193E-09	1.10E-6	105503.58%	105473.03%
8	14.22374	14.22376	3.69E-09	3.68933E-09	1.00E-6	27004.15%	27005.18%
9	11.59798	11.59826	3.11E-07	3.10984E-07	4.00E-5	12756.37%	12762.40%
10	10.11471	10.11545	3.81E-06	3.80511E-06	5.50E-4	14336.16%	14354.23%
11	7.501853	7.501876	0.000314	0.000314349	1.40E-2	4353.48%	4353.65%
12	30.84445	30.84397	2.38E-21	2.37742E-21	0	0%	0%
13 CDCl3	-6.30457	-6.30396	99.99763	99.99762279	86	14.00%	14.00%

13 DMSO	-6.30457	-6.30396	99.99763	99.99762279	63	37.00%	37.00%
13	-6.30457	-6.30396	99.99763	99.99762279	80	20.00%	20.00%
14 CDCl3	N/A	N/A	N/A	N/A	3	N/A	N/A
14 DMSO	N/A	N/A	N/A	N/A	0	N/A	N/A
14	N/A	N/A	N/A	N/A	8	N/A	N/A
15 CDCl3	N/A	N/A	N/A	N/A	85	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99	N/A	N/A
15	N/A	N/A	N/A	N/A	89	N/A	N/A
16	-4.53684	-4.53689	99.95301	99.95300973	80	19.96%	19.96%
17	-6.45444	-6.45394	99.99816	99.99815471	91.7	8.30%	8.30%
18	-7.82915	-7.82944	99.99982	99.99981922	91.7	8.30%	8.30%
19	-7.50935	-7.50941	99.99969	99.99968962	95.8	4.20%	4.20%
20	5.908326	5.908629	0.004637	0.004634799	95.3	2055030.17%	2056083.95%
21	N/A	N/A	N/A	N/A	98	N/A	N/A
22	-5.18374	-5.18386	99.98424	99.9842384	82.1	17.89%	17.89%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A

24	-6.92858	-6.92833	99.99917	99.99917187	93.4	6.60%	6.60%
25	6.957891	6.957825	0.000788	0.000787894	91.6	11627116.05%	11625825.80%
26	-6.49939	-6.49974	99.99829	99.99829209	93.7	6.30%	6.30%
27	-5.8733	-5.87286	99.99508	99.9950766	85.2	14.80%	14.80%
28	-4.67217	-4.67244	99.9626	99.96262077	88.5	11.47%	11.47%
29	-5.54286	-5.54279	99.9914	99.99140286	89.2	10.79%	10.79%
30	N/A	N/A	N/A	N/A	90.8	N/A	N/A
31	-6.56065	-6.55998	99.99846	99.99845731	93.4	6.60%	6.60%
32	-5.23939	-5.24033	99.98565	99.98567213	93.7	6.29%	6.29%
33	-5.15023	-5.14997	99.98332	99.98331021	94.6	5.38%	5.38%
34	-5.58919	-5.58923	99.99205	99.99205129	93.9	6.09%	6.09%
35	-5.45773	-5.45808	99.99007	99.9900806	95.9	4.09%	4.09%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A

40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-4.64349	-4.6442	99.96075	99.9607956	40.5	59.48%	59.48%
42 CDCl3	-6.90033	-6.90072	99.99913	99.99913233	92.6	7.40%	7.40%
43 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	-7.60685	-7.6073	99.99974	99.99973692	90.2	9.80%	9.80%
44 Acetone	-7.60685	-7.6073	99.99974	99.99973692	93.6	6.40%	6.40%
44 CDCl3	-7.60685	-7.6073	99.99974	99.99973692	91.6	8.40%	8.40%
45 DMSO	-6.85055	-6.85052	99.99906	99.99905556	94.6	5.40%	5.40%
45Acetone	-6.85055	-6.85052	99.99906	99.99905556	99.3	0.70%	0.70%
45 CDCl3	-6.85055	-6.85052	99.99906	99.99905556	97.3	2.70%	2.70%
46 DMSO	-5.98578	-5.98581	99.99593	99.99593164	93.7	6.30%	6.30%
46 Acetone	-5.98578	-5.98581	99.99593	99.99593164	97.3	2.70%	2.70%
46 CDCl3	-5.98578	-5.98581	99.99593	99.99593164	95.7	4.30%	4.30%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A

47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-5.83391	-5.83333	99.99474	99.99473666	94.6	5.40%	5.40%
50 Acetone	-5.83391	-5.83333	99.99474	99.99473666	97.8	2.19%	2.19%
50 CDCl3	-5.83391	-5.83333	99.99474	99.99473666	97.2	2.79%	2.79%
51 DMSO	-5.8642	-5.86408	99.995	99.99500301	94	6.00%	6.00%
51 Acetone	-5.8642	-5.86408	99.995	99.99500301	96.4	3.60%	3.60%
51 CDCl3	-5.8642	-5.86408	99.995	99.99500301	96.1	3.90%	3.90%
52 DMSO	-5.98065	-5.98079	99.9959	99.995897	95	5.00%	5.00%
52 Acetone	-5.98065	-5.98079	99.9959	99.995897	96.7	3.30%	3.30%

52 CDCl3	-5.98065	-5.98079	99.9959	99.995897	97.9	2.10%	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						2.79E3%	2.79E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.41%	12.40%

Table 1.24: Convergence results M05-2X 6-31G gas phase and how it compares to experimental data.

1.5.5 M05-2X cc-pVDZ

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-3.01287	-3.0133	99.38707	99.38752052	41.7	58.04%	58.04%
2 ethanol	-47190.6	-47190.6	N/A	N/A	44.1	N/A	N/A
3 ethanol	-2.28208	-2.28225	97.92507	97.92567604	44.1	54.97%	54.97%
4 ethanol	-2.40379	-2.40336	98.30409	98.30287758	48.3	50.87%	50.87%
5 ethanol	-2.7429	-2.74347	99.03641	99.03733131	47.6	51.94%	51.94%
6	14.56648	14.56638	2.07E-09	2.06841E-09	6.00E-7	28912.93%	28907.73%
7	14.24402	14.24384	3.57E-09	3.56631E-09	1.10E-6	30753.94%	30744.22%
8	13.33609	13.33583	1.65E-08	1.65286E-08	1.00E-6	5952.78%	5950.11%
9	11.02771	11.02785	8.15E-07	8.14944E-07	4.00E-5	4807.09%	4808.31%
10	9.370837	9.371227	1.34E-05	1.33738E-05	5.50E-4	4009.82%	4012.53%
11	7.180492	7.180591	0.000541	0.000540843	1.40E-2	2488.12%	2488.55%
12	29.82934	29.82929	1.32E-20	1.31938E-20	0	0%	0%
13 CDCl3	-7.06895	-7.06889	99.99935	99.99934687	86	14.00%	14.00%

13 DMSO	-7.06895	-7.06889	99.99935	99.99934687	63	37.00%	37.00%
13	-7.06895	-7.06889	99.99935	99.99934687	80	20.00%	20.00%
14 CDCl3	-4.19356	-4.19365	99.91612	99.91612779	3	97.00%	97.00%
14 DMSO	-4.19356	-4.19365	99.91612	99.91612779	0	0%	0%
14	-4.19356	-4.19365	99.91612	99.91612779	8	91.99%	91.99%
15 CDCl3	-6.30387	-6.30396	99.99762	99.99762279	85	15.00%	15.00%
15 DMSO	-6.30387	-6.30396	99.99762	99.99762279	99	1.00%	1.00%
15	-6.30387	-6.30396	99.99762	99.99762279	89	11.00%	11.00%
16	-4.98335	-4.98368	99.97789	99.97789959	80	19.98%	19.98%
17	-6.49997	-6.49974	99.99829	99.99829209	91.7	8.30%	8.30%
18	-8.21381	-8.21347	99.99991	99.99990549	91.7	8.30%	8.30%
19	-7.34972	-7.34939	99.99959	99.99959332	95.8	4.20%	4.20%
20	4.988704	4.988701	0.021914	0.021913864	95.3	434787.39%	434784.51%
21	-6.95325	-6.95343	99.99921	99.99920624	98	2.00%	2.00%
22	-5.93181	-5.93185	99.99554	99.99554342	82.1	17.90%	17.90%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A

24	-8.12209	-8.12186	99.99989	99.99988968	93.4	6.60%	6.60%
25	6.927604	6.927077	0.000829	0.000829891	91.6	11047310.25%	11037489.97%
26	-7.51717	-7.51756	99.99969	99.99969387	93.7	6.30%	6.30%
27	-6.53678	-6.53677	99.9984	99.99839561	85.2	14.80%	14.80%
28	-5.34867	-5.34889	99.98807	99.98807209	88.5	11.49%	11.49%
29	-6.21827	-6.21799	99.99725	99.99725132	89.2	10.80%	10.80%
30	-5.69558	-5.6959	99.99336	99.99336172	90.8	9.19%	9.19%
31	-7.25536	-7.25589	99.99952	99.99952375	93.4	6.60%	6.60%
32	-7.76588	-7.76543	99.9998	99.99979858	93.7	6.30%	6.30%
33	-5.73382	-5.73418	99.99377	99.99377728	94.6	5.39%	5.39%
34	-6.63463	-6.63403	99.99864	99.99863866	93.9	6.10%	6.10%
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A

40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-5.36553	-5.36583	99.9884	99.98840853	40.5	59.50%	59.50%
42 CDCl3	-7.60278	-7.60291	99.99973	99.99973496	92.6	7.40%	7.40%
43 DMSO	-7.4003	-7.39959	99.99963	99.99962637	94	6.00%	6.00%
43 Acetone	-7.4003	-7.39959	99.99963	99.99962637	97.7	2.30%	2.30%
43 CDCl3	-7.4003	-7.39959	99.99963	99.99962637	97.8	2.20%	2.20%
44 DMSO	-8.5255	-8.52534	99.99994	99.99994419	90.2	9.80%	9.80%
44 Acetone	-8.5255	-8.52534	99.99994	99.99994419	93.6	6.40%	6.40%
44 CDCl3	-8.5255	-8.52534	99.99994	99.99994419	91.6	8.40%	8.40%
45 DMSO	-7.55483	-7.55459	99.99971	99.99971243	94.6	5.40%	5.40%
45Acetone	-7.55483	-7.55459	99.99971	99.99971243	99.3	0.70%	0.70%
45 CDCl3	-7.55483	-7.55459	99.99971	99.99971243	97.3	2.70%	2.70%
46 DMSO	-7.29515	-7.29543	99.99955	99.99955451	93.7	6.30%	6.30%
46 Acetone	-7.29515	-7.29543	99.99955	99.99955451	97.3	2.70%	2.70%
46 CDCl3	-7.29515	-7.29543	99.99955	99.99955451	95.7	4.30%	4.30%
47 DMSO	-8.60891	-8.6088	99.99995	99.99995153	70.1	29.90%	29.90%

47 Acetone	-8.60891	-8.6088	99.99995	99.99995153	87.1	12.90%	12.90%
47 CDCl3	-8.60891	-8.6088	99.99995	99.99995153	86.6	13.40%	13.40%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	-7.27359	-7.27284	99.99954	99.99953718	95	5.00%	5.00%
52 Acetone	-7.27359	-7.27284	99.99954	99.99953718	96.7	3.30%	3.30%

52 $CDCl_3$	-7.27359	-7.27284	99.99954	99.99953718	97.9	2.10%	2.10%
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.99E3%	1.99E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						16.75%	16.75%

Table 1.25: Convergence results M05-2X cc-pVDZ gas phase and how it compares to experimental data.

1.6 M06 gas phase

1.6.1 M06 6-311++ G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.92025	-0.92056	82.55263	82.56000493	41.7	49.49%	49.49%
2 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
3 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
4 ethanol	-0.34102	-0.34137	64.01368	64.02716321	48.3	24.55%	24.56%
5 ethanol	-1.22855	-1.22866	88.84442	88.84625359	47.6	46.42%	46.42%
6	15.7098	15.71033	3E-10	2.9961E-10	6E-7	199980.50%	200160.32%
7	16.1314	16.13139	1.47E-10	1.47134E-10	1.1E-6	747539.13%	747519.87%
8	15.2835	15.28362	6.16E-10	6.15947E-10	1E-6	162217.06%	162251.65%
9	12.93551	12.93548	3.25E-08	3.25007E-08	4E-5	122981.05%	122974.43%
10	11.3968	11.39683	4.37E-07	4.37005E-07	5.5E-4	125751.05%	125756.70%
11	8.19175	8.192137	9.8E-05	9.79738E-05	1.4E-2	14180.21%	14189.53%
12	32.81741	32.81686	8.48E-23	8.49182E-23	0	0.00%	0.00%
13 CDCl3	-2.34082	-2.34061	98.11737	98.1167091	86.0	12.35%	12.35%
13 DMSO	-2.34082	-2.34061	98.11737	98.1167091	63.0	35.79%	35.79%
13	-2.34082	-2.34061	98.11737	98.1167091	80.0	18.46%	18.46%
14 CDCl3	-0.60039	-0.60053	73.38053	73.38510342	3.0	95.91%	95.91%

14 DMSO	-0.60039	-0.60053	73.38053	73.38510342	0	0.00%	0.00%
14	-0.60039	-0.60053	73.38053	73.38510342	8.0	89.10%	89.10%
15 CDCl3	N/A	N/A	N/A	N/A	85.0	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99.0	N/A	N/A
15	N/A	N/A	N/A	N/A	89.0	N/A	N/A
16	0.083611	0.083459	46.47553	46.48191411	80.0	72.13%	72.11%
17	-2.13658	-2.1373	97.36234	97.36543849	91.7	5.82%	5.82%
18	-3.7413	-3.74121	99.82011	99.82008859	91.7	8.13%	8.13%
19	N/A	N/A	N/A	N/A	95.8	N/A	N/A
20	N/A	N/A	N/A	N/A	95.3	N/A	N/A
21	-3.94714	-3.94703	99.87287	99.87284952	98.0	1.88%	1.88%
22	N/A	N/A	N/A	N/A	82.1	N/A	N/A
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-3.29388	-3.2938	99.6178	99.61774472	93.4	6.24%	6.24%
25	8.04859	8.048437	0.000125	0.000124886	91.6	73365849.92%	73346929.74%
26	-3.08127	-3.0817	99.45359	99.45397583	93.7	5.79%	5.79%
27	-1.78971	-1.79028	95.35895	95.36322018	85.2	10.65%	10.66%
28	-1.63054	-1.6309	94.01318	94.01657529	88.5	5.86%	5.87%
29	N/A	N/A	N/A	N/A	89.2	N/A	N/A
30	-1.26119	-1.26129	89.37913	89.38080466	90.8	1.59%	1.59%

31	-3.48154	-3.48142	99.72133	99.72127086	93.4	6.34%	6.34%
32	-3.20133	-3.20093	99.55342	99.55311853	93.7	5.88%	5.88%
33	-5.62242	-5.62249	99.99248	99.99248544	94.6	5.39%	5.39%
34	-1.57829	-1.57819	93.49677	93.49570598	93.9	0.43%	0.43%
35	-1.64953	-1.64972	94.19121	94.19295015	95.9	1.81%	1.81%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	N/A	N/A	N/A	N/A	40.5	N/A	N/A
42 CDCl3	-2.98208	-2.98193	99.35458	99.3544044	92.6	6.80%	6.80%
43 DMSO	-2.97449	-2.9744	99.34629	99.3461954	94.0	5.38%	5.38%
43 Acetone	-2.97449	-2.9744	99.34629	99.3461954	97.7	1.66%	1.66%
43 CDCl3	-2.97449	-2.9744	99.34629	99.3461954	97.8	1.56%	1.56%
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-3.14552	-3.14571	99.50949	99.50964922	94.6	4.93%	4.93%
45Acetone	-3.14552	-3.14571	99.50949	99.50964922	99.3	0.21%	0.21%

45 CDCl3	-3.14552	-3.14571	99.50949	99.50964922	97.3	2.22%	2.22%
46 DMSO	N/A	N/A	N/A	N/A	93.7	N/A	N/A
46 Acetone	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 CDCl3	N/A	N/A	N/A	N/A	95.7	N/A	N/A
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92.0	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	13.00041	13.00011	2.91E-08	2.91396E-08	94.0	322745539436.30%	322584876911.74%
51 Acetone	13.00041	13.00011	2.91E-08	2.91396E-08	96.4	330985851084.04%	330821086537.57%

51 CDCl3	13.00041	13.00011	2.91E-08	2.91396E-08	96.1	329955812128.07 %	329791560334. 34%
52 DMSO	N/A	N/A	N/A	N/A	95.0	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						2.40E8%	2.40E8%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						17.19%	17.19%

Table 1.26: Convergence results from M06-6-311++G gas phase and how it compares to experimental data.

1.6.2 M06 6-31++ G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	N/A	N/A	N/A	N/A	41.7	N/A	N/A
2 ethanol	-47175	-47175	N/A	N/A	44.1	N/A	N/A
3 ethanol	0.705079	0.705321	23.31102	23.30372008	44.1	89.18%	89.24%
4 ethanol	-0.46052	-0.46059	68.52023	68.52293937	48.3	29.51%	29.51%
5 ethanol	-1.08488	-1.08434	86.20353	86.19251888	47.6	44.78%	44.77%
6	16.42538	16.42569	8.96E-11	8.95041E-11	6E-7	669905.60%	670260.41%
7	16.51076	16.51103	7.75E-11	7.749E-11	1.1E-6	1418779.53%	1419438.52%
8	15.72076	15.721	2.94E-10	2.9426E-10	1E-6	339599.15%	339735.18%
9	13.1934	13.19339	2.1E-08	2.10242E-08	4E-5	190160.71%	190157.08%
10	11.60364	11.60391	3.08E-07	3.08032E-07	5.5E-4	178371.68%	178452.97%
11	8.084683	8.084832	0.000117	0.00011744	1.4E-2	11817.95%	11820.95%
12	33.10195	33.10175	5.25E-23	5.24851E-23	0	0%	0%
13 CDCl3	-2.54128	-2.54204	98.65078	98.65248317	86.0	12.82%	12.83%
13 DMSO	-2.54128	-2.54204	98.65078	98.65248317	63.0	36.14%	36.14%
13	-2.54128	-2.54204	98.65078	98.65248317	80.0	18.91%	18.91%
14 CDCl3	N/A	N/A	N/A	N/A	3.0	N/A	N/A
14 DMSO	N/A	N/A	N/A	N/A	0	N/A	N/A

14	N/A	N/A	N/A	N/A	8.0	N/A	N/A
15 CDCl3	-3.57653	-3.5768	99.76253	99.76264372	85.0	14.80%	14.80%
15 DMSO	-3.57653	-3.5768	99.76253	99.76264372	99.0	0.76%	0.76%
15	-3.57653	-3.5768	99.76253	99.76264372	89.0	10.79%	10.79%
16	N/A	N/A	N/A	N/A	80.0	N/A	N/A
17	N/A	N/A	N/A	N/A	91.7	N/A	N/A
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	N/A	N/A	N/A	N/A	95.8	N/A	N/A
20	6.656599	6.655993	0.00131	0.001311771	95.3	7272323.60%	7264889.61%
21	-4.75071	-4.75025	99.96725	99.96722247	98.0	1.97%	1.97%
22	-2.06424	-2.06451	97.02976	97.03102837	82.1	15.39%	15.39%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-2.84507	-2.84513	99.18789	99.18796944	93.4	5.84%	5.84%
25	7.69441	7.695149	0.000227	0.000226802	91.6	40337129.22%	40387512.13%
26	-3.83889	-3.8391	99.84741	99.84746311	93.7	6.16%	6.16%
27	-0.77993	-0.77999	78.87244	78.87419847	85.2	8.02%	8.02%
28	-2.46789	-2.46737	98.47544	98.47411785	88.5	10.13%	10.13%
29	-2.96282	-2.9631	99.33337	99.33368707	89.2	10.20%	10.20%
30	-2.19448	-2.1944	97.60217	97.6018489	90.8	6.97%	6.97%
31	N/A	N/A	N/A	N/A	93.4	N/A	N/A

32	-2.25999	-2.25966	97.84791	97.84674101	93.7	4.24%	4.24%
33	-6.37893	-6.37926	99.99791	99.99790668	94.6	5.40%	5.40%
34	-2.31376	-2.31363	98.03106	98.03062674	93.9	4.21%	4.21%
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	N/A	N/A	N/A	N/A	40.5	N/A	N/A
42 CDCl3	-4.27099	-4.27083	99.92639	99.92637102	92.6	7.33%	7.33%
43 DMSO	-3.58201	-3.58182	99.76472	99.76464294	94.0	5.78%	5.78%
43 Acetone	-3.58201	-3.58182	99.76472	99.76464294	97.7	2.07%	2.07%
43 CDCl3	-3.58201	-3.58182	99.76472	99.76464294	97.8	1.97%	1.97%
44 DMSO	-5.1534	-5.15374	99.98341	99.98341598	90.2	9.79%	9.79%
44 Acetone	-5.1534	-5.15374	99.98341	99.98341598	93.6	6.38%	6.38%
44 CDCl3	-5.1534	-5.15374	99.98341	99.98341598	91.6	8.38%	8.38%
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A
45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A

46 DMSO	-3.89586	-3.89621	99.86139	99.86146779	93.7	6.17%	6.17%
46 Acetone	-3.89586	-3.89621	99.86139	99.86146779	97.3	2.56%	2.57%
46 CDCl3	-3.89586	-3.89621	99.86139	99.86146779	95.7	4.17%	4.17%
47 DMSO	-4.56793	-4.56827	99.95541	99.95543389	70.1	29.87%	29.87%
47 Acetone	-4.56793	-4.56827	99.95541	99.95543389	87.1	12.86%	12.86%
47 CDCl3	-4.56793	-4.56827	99.95541	99.95543389	86.6	13.36%	13.36%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	-3.97886	-3.97904	99.8795	99.87953163	82.5	17.40%	17.40%
49 Acetone	-3.97886	-3.97904	99.8795	99.87953163	92.0	7.89%	7.89%
49 CDCl3	-3.97886	-3.97904	99.8795	99.87953163	88.2	11.69%	11.69%
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	-3.29034	-3.29003	99.61551	99.61531562	95.0	4.63%	4.63%
52 Acetone	-3.29034	-3.29003	99.61551	99.61531562	96.7	2.93%	2.93%

52 CDCl3	-3.29034	-3.29003	99.61551	99.61531562	97.9	1.72%	1.72%
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.05E4%	1.05E4%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.33%	12.33%

Table 1.27: Convergence results from M06-6-31++G gas phase and how it compares to experimental data.

1.6.3 M06 6-31+G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-0.83856	-0.83835	80.4753	80.4698399	41.7	48.18%	48.18%
2 ethanol	-47174.9	-47174.9	N/A	N/A	44.1	N/A	N/A
3 ethanol	-1.27864	-1.27886	89.65563	89.65919206	44.1	50.81%	50.81%
4 ethanol	-0.40329	-0.40286	66.39897	66.38292791	48.3	27.26%	27.24%
5 ethanol	N/A	N/A	N/A	N/A	47.6	N/A	N/A
6	16.54812	16.54805	7.28E-11	7.27929E-11	6E-7	824245.34%	824155.72%
7	16.55408	16.5537	7.21E-11	7.21019E-11	1.1E-6	1526498.93%	1525518.27%
8	15.8419	15.84273	2.4E-10	2.39573E-10	1E-6	416724.13%	417308.87%
9	13.3151	13.31512	1.71E-08	1.71169E-08	4E-5	233576.05%	233586.79%
10	11.67202	11.67168	2.75E-07	2.74717E-07	5.5E-4	200222.19%	200105.85%
11	8.348882	8.348386	7.52E-05	7.52492E-05	1.4E-2	18520.45%	18504.86%
12	33.26829	33.26867	3.96E-23	3.95916E-23	0	0%	0%
13 CDCl3	-2.46238	-2.46235	98.4614	98.46132544	86.0	12.66%	12.66%
13 DMSO	-2.46238	-2.46235	98.4614	98.46132544	63.0	36.02%	36.02%
13	-2.46238	-2.46235	98.4614	98.46132544	80.0	18.75%	18.75%
14 CDCl3	-0.85537	-0.8553	80.9176	80.91563589	3.0	96.29%	96.29%
14 DMSO	-0.85537	-0.8553	80.9176	80.91563589	0	0%	0%

14	-0.85537	-0.8553	80.9176	80.91563589	8.0	90.11%	90.11%
15 CDCl3	-2.43101	-2.43034	98.37906	98.3772567	85.0	13.60%	13.60%
15 DMSO	-2.43101	-2.43034	98.37906	98.3772567	99.0	0.63%	0.63%
15	-2.43101	-2.43034	98.37906	98.3772567	89.0	9.53%	9.53%
16	-0.46673	-0.46561	68.74602	68.70552604	80.0	16.37%	16.44%
17	N/A	N/A	N/A	N/A	91.7	N/A	N/A
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-4.66705	-4.66742	99.96228	99.96230262	95.8	4.16%	4.16%
20	6.203217	6.203559	0.002818	0.002816499	95.3	3381579.58%	3383533.32%
21	-4.76646	-4.76656	99.96811	99.96811305	98.0	1.97%	1.97%
22	-2.04512	-2.04568	96.93526	96.93805105	82.1	15.30%	15.31%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-3.68554	-3.68599	99.80238	99.80253664	93.4	6.42%	6.42%
25	N/A	N/A	N/A	N/A	91.6	N/A	N/A
26	-3.78527	-3.78576	99.83297	99.83310789	93.7	6.14%	6.14%
27	N/A	N/A	N/A	N/A	85.2	N/A	N/A
28	-2.41782	-2.41842	98.34314	98.34479526	88.5	10.01%	10.01%
29	N/A	N/A	N/A	N/A	89.2	N/A	N/A
30	-2.16516	-2.16554	97.48349	97.48505108	90.8	6.86%	6.86%
31	N/A	N/A	N/A	N/A	93.4	N/A	N/A

32	-4.06752	-4.06752	99.89624	99.89623595	93.7	6.20%	6.20%
33	-6.5643	-6.56375	99.99847	99.99846709	94.6	5.40%	5.40%
34	-2.39153	-2.39207	98.26922	98.27075636	93.9	4.45%	4.45%
35	-5.07807	-5.07906	99.98116	99.98118723	95.9	4.08%	4.08%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	N/A	N/A	N/A	N/A	40.5	N/A	N/A
42 CDCl3	-4.25607	-4.25577	99.92451	99.92447562	92.6	7.33%	7.33%
43 DMSO	-2.97473	-2.97502	99.34656	99.34688342	94.0	5.38%	5.38%
43 Acetone	-2.97473	-2.97502	99.34656	99.34688342	97.7	1.66%	1.66%
43 CDCl3	-2.97473	-2.97502	99.34656	99.34688342	97.8	1.56%	1.56%
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-3.99549	-3.99473	99.88283	99.8826779	94.6	5.29%	5.29%
45Acetone	-3.99549	-3.99473	99.88283	99.8826779	99.3	0.58%	0.58%
45 CDCl3	-3.99549	-3.99473	99.88283	99.8826779	97.3	2.59%	2.59%

46 DMSO	12.50545	12.50564	6.72E-08	6.71708E-08	93.7	139450716205.82 %	139495140818. 13%
46 Acetone	12.50545	12.50564	6.72E-08	6.71708E-08	97.3	144808481186.62 %	144854612614. 34%
46 CDCl3	12.50545	12.50564	6.72E-08	6.71708E-08	95.7	142427252306.27 %	142472625149. 36%
47 DMSO	-4.58239	-4.5827	99.95648	99.95650663	70.1	29.87%	29.87%
47 Acetone	-4.58239	-4.5827	99.95648	99.95650663	87.1	12.86%	12.86%
47 CDCl3	-4.58239	-4.5827	99.95648	99.95650663	86.6	13.36%	13.36%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	-4.76687	-4.76719	99.96813	99.96814682	82.5	17.47%	17.47%
49 Acetone	-4.76687	-4.76719	99.96813	99.96814682	92.0	7.97%	7.97%
49 CDCl3	-4.76687	-4.76719	99.96813	99.96814682	88.2	11.77%	11.77%
50 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
50 Acetone	N/A	N/A	N/A	N/A	97.8	N/A	N/A
50 CDCl3	N/A	N/A	N/A	N/A	97.2	N/A	N/A
51 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A

51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95.0	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						8.89E7%	8.89E7%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						16.02%	16.03%

Table 1.28: Convergence results from M06 6-31+G gas phase and how it compares to experimental data.

1.6.4 M06 6-31G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-1.36401	-1.36358	90.91845	90.91246748	41.7	54.13%	54.13%
2 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
3 ethanol	-1.47134	-1.47088	92.30827	92.30283893	44.1	52.23%	52.22%
4 ethanol	-0.77491	-0.77497	78.73064	78.73257571	48.3	38.65%	38.65%
5 ethanol	-1.15687	-1.1565	87.58693	87.58008488	47.6	45.65%	45.65%
6	17.11647	17.11658	2.79E-11	2.78664E-11	6E-7	2152652.68%	2153034.08%
7	17.86409	17.86457	7.88E-12	7.8783E-12	1.1E-6	13950988.31%	13962305.65%
8	16.52166	16.5217	7.61E-11	7.61063E-11	1E-6	1313769.98%	1313851.01%
9	14.02083	14.02107	5.2E-09	5.19537E-09	4E-5	769502.88%	769816.25%
10	12.91732	12.91728	3.35E-08	3.35151E-08	5.5E-4	1641052.13%	1640952.77%
11	10.10863	10.10855	3.85E-06	3.84973E-06	1.4E-2	363613.24%	363561.42%
12	34.04341	34.04365	1.07E-23	1.06946E-23	0	0.00%	0.00%
13 CDCl3	-3.92806	-3.92758	99.86871	99.86860825	86.0	13.89%	13.89%
13 DMSO	-3.92806	-3.92758	99.86871	99.86860825	63.0	36.92%	36.92%
13	-3.92806	-3.92758	99.86871	99.86860825	80.0	19.89%	19.89%
14 CDCl3	-0.94463	-0.94503	83.13761	83.14715204	3.0	96.39%	96.39%
14 DMSO	-0.94463	-0.94503	83.13761	83.14715204	0	0.00%	0.00%

14	-0.94463	-0.94503	83.13761	83.14715204	8.0	90.38%	90.38%
15 CDCl3	-4.35759	-4.35743	99.9364	99.93638283	85.0	14.95%	14.95%
15 DMSO	-4.35759	-4.35743	99.9364	99.93638283	99.0	0.94%	0.94%
15	-4.35759	-4.35743	99.9364	99.93638283	89.0	10.94%	10.94%
16	-1.58453	-1.58509	93.56057	93.56624282	80.0	14.49%	14.50%
17	-3.08052	-3.08044	99.45289	99.45282356	91.7	7.80%	7.80%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-4.792	-4.79229	99.96945	99.96946854	95.8	4.17%	4.17%
20	N/A	N/A	N/A	N/A	95.3	N/A	N/A
21	-3.55489	-3.55484	99.75372	99.75369604	98.0	1.76%	1.76%
22	-4.89876	-4.89834	99.97449	99.97447399	82.1	17.88%	17.88%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-4.45573	-4.45532	99.94611	99.94607209	93.4	6.55%	6.55%
25	8.373788	8.374742	7.21E-05	7.19731E-05	91.6	127064724.43%	127269674.85%
26	-4.16736	-4.16729	99.91232	99.91231343	93.7	6.22%	6.22%
27	-2.65435	-2.65374	98.88269	98.88156037	85.2	13.84%	13.84%
28	N/A	N/A	N/A	N/A	88.5	N/A	N/A
29	N/A	N/A	N/A	N/A	89.2	N/A	N/A
30	-2.22241	-2.22264	97.71012	97.71098048	90.8	7.07%	7.07%
31	-2.05959	-2.06011	97.00701	97.00958152	93.4	3.72%	3.72%

32	-2.44969	-2.4498	98.42861	98.42888079	93.7	4.80%	4.80%
33	-6.11914	-6.11885	99.99675	99.99675029	94.6	5.40%	5.40%
34	-3.04884	-3.04844	99.423	99.42260975	93.9	5.56%	5.55%
35	-3.1504	-3.15135	99.5135	99.51428154	95.9	3.63%	3.63%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-2.4759	-2.47615	98.49563	98.49625307	40.5	58.88%	58.88%
42 CDCl3	-4.97295	-4.97239	99.9775	99.97747403	92.6	7.38%	7.38%
43 DMSO	-3.49495	-3.4946	99.72755	99.72738908	94.0	5.74%	5.74%
43 Acetone	-3.49495	-3.4946	99.72755	99.72738908	97.7	2.03%	2.03%
43 CDCl3	-3.49495	-3.4946	99.72755	99.72738908	97.8	1.93%	1.93%
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-3.6708	-3.67093	99.79741	99.7974599	94.6	5.21%	5.21%
45Acetone	-3.6708	-3.67093	99.79741	99.7974599	99.3	0.50%	0.50%
45 CDCl3	-3.6708	-3.67093	99.79741	99.7974599	97.3	2.50%	2.50%

46 DMSO	N/A	N/A	N/A	N/A	93.7	N/A	N/A
46 Acetone	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 CDCl3	N/A	N/A	N/A	N/A	95.7	N/A	N/A
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	-4.64267	-4.64294	99.96069	99.96071245	82.5	17.47%	17.47%
49 Acetone	-4.64267	-4.64294	99.96069	99.96071245	92.0	7.96%	7.96%
49 CDCl3	-4.64267	-4.64294	99.96069	99.96071245	88.2	11.77%	11.77%
50 DMSO	-5.08754	-5.08722	99.98145	99.9814446	94.6	5.38%	5.38%
50 Acetone	-5.08754	-5.08722	99.98145	99.9814446	97.8	2.18%	2.18%
50 CDCl3	-5.08754	-5.08722	99.98145	99.9814446	97.2	2.78%	2.78%
51 DMSO	-3.56286	-3.56237	99.757	99.75680109	94.0	5.77%	5.77%
51 Acetone	-3.56286	-3.56237	99.757	99.75680109	96.4	3.37%	3.36%
51 CDCl3	-3.56286	-3.56237	99.757	99.75680109	96.1	3.67%	3.67%
52 DMSO	N/A	N/A	N/A	N/A	95.0	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A

52 $CDCl_3$	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						2.83E4%	2.84E4%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						16.05%	16.05%

Table 1.29: Convergence results from M06 6-31G gas phase and how it compares to experimental data.

1.6.5 M06 cc-pVDZ

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-1.16322	-1.16278	87.70305	87.69490729	41.7	52.45%	52.45%
2 ethanol	-47176.2	-47176.2	N/A	N/A	44.1	N/A	N/A
3 ethanol	-2.31961	-2.31928	98.05005	98.04895735	44.1	55.02%	55.02%
4 ethanol	-2.28574	-2.28602	97.9376	97.93855363	48.3	50.68%	50.68%
5 ethanol	-0.91987	-0.9193	82.54329	82.52946425	47.6	42.33%	42.32%
6	17.68872	17.68887	1.06E-11	1.06001E-11	6E-7	5658808.36%	5660231.03%
7	16.8403	16.84047	4.44E-11	4.44223E-11	1.1E-6	2475425.03%	2476133.14%
8	15.54597	15.54655	3.95E-10	3.95083E-10	1E-6	252763.25%	253011.51%
9	13.18309	13.18335	2.14E-08	2.13837E-08	4E-5	186876.68%	186958.06%
10	12.24895	12.24899	1.04E-07	1.03617E-07	5.5E-4	530668.77%	530698.55%
11	9.85852	9.858174	5.87E-06	5.87598E-06	1.4E-2	238297.29%	238158.02%
12	32.80282	32.80306	8.7E-23	8.69214E-23	0	0.00%	0.00%
13 CDCl3	-4.35667	-4.35617	99.9363	99.93624792	86.0	13.95%	13.95%
13 DMSO	-4.35667	-4.35617	99.9363	99.93624792	63.0	36.96%	36.96%
13	-4.35667	-4.35617	99.9363	99.93624792	80.0	19.95%	19.95%
14 CDCl3	-1.92419	-1.92394	96.26668	96.26520853	3.0	96.88%	96.88%
14 DMSO	-1.92419	-1.92394	96.26668	96.26520853	0	0.00%	0.00%

14	-1.92419	-1.92394	96.26668	96.26520853	8.0	91.69%	91.69%
15 CDCl3	-3.13768	-3.13818	99.50299	99.50340435	85.0	14.58%	14.58%
15 DMSO	-3.13768	-3.13818	99.50299	99.50340435	99.0	0.51%	0.51%
15	-3.13768	-3.13818	99.50299	99.50340435	89.0	10.56%	10.56%
16	N/A	N/A	N/A	N/A	80.0	N/A	N/A
17	-3.39903	-3.39922	99.67979	99.67989081	91.7	8.01%	8.01%
18	-5.9891	-5.98895	99.99595	99.99595314	91.7	8.30%	8.30%
19	-4.83024	-4.83057	99.97136	99.97137937	95.8	4.17%	4.17%
20	4.586206	4.586467	0.043237	0.0432178	95.3	220313.88%	220410.99%
21	N/A	N/A	N/A	N/A	98.0	N/A	N/A
22	N/A	N/A	N/A	N/A	82.1	N/A	N/A
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-5.25706	-5.25727	99.98607	99.98607626	93.4	6.59%	6.59%
25	7.762241	7.76292	0.000203	0.000202273	91.6	45233376.48%	45285253.79%
26	-4.45717	-4.45657	99.94624	99.94618622	93.7	6.25%	6.25%
27	-3.14344	-3.14382	99.50778	99.50809537	85.2	14.38%	14.38%
28	-2.69536	-2.69578	98.95669	98.95742526	88.5	10.57%	10.57%
29	N/A	N/A	N/A	N/A	89.2	N/A	N/A
30	-2.75452	-2.75351	99.05495	99.05336458	90.8	8.33%	8.33%
31	-2.8633	-2.86333	99.21231	99.21235385	93.4	5.86%	5.86%

32	-3.31455	-3.31451	99.63086	99.63083419	93.7	5.95%	5.95%
33	-7.17112	-7.17055	99.99945	99.99944991	94.6	5.40%	5.40%
34	-4.09766	-4.09764	99.90138	99.90137749	93.9	6.01%	6.01%
35	-4.17116	-4.17106	99.91288	99.91286877	95.9	4.02%	4.02%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-2.68254	-2.6826	98.93411	98.93421137	40.5	59.06%	59.06%
42 CDCl3	N/A	N/A	N/A	N/A	92.6	N/A	N/A
43 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	N/A	N/A	N/A	N/A	94.6	N/A	N/A
45Acetone	N/A	N/A	N/A	N/A	99.3	N/A	N/A
45 CDCl3	N/A	N/A	N/A	N/A	97.3	N/A	N/A

46 DMSO	N/A	N/A	N/A	N/A	93.7	N/A	N/A
46 Acetone	N/A	N/A	N/A	N/A	97.3	N/A	N/A
46 CDCl3	N/A	N/A	N/A	N/A	95.7	N/A	N/A
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92.0	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-6.17487	-6.17532	99.99704	99.99704593	94.6	5.40%	5.40%
50 Acetone	-6.17487	-6.17532	99.99704	99.99704593	97.8	2.20%	2.20%
50 CDCl3	-6.17487	-6.17532	99.99704	99.99704593	97.2	2.80%	2.80%
51 DMSO	-5.97684	-5.97703	99.99587	99.99587083	94.0	6.00%	6.00%
51 Acetone	-5.97684	-5.97703	99.99587	99.99587083	96.4	3.60%	3.60%
51 CDCl3	-5.97684	-5.97703	99.99587	99.99587083	96.1	3.90%	3.90%
52 DMSO	-5.34105	-5.34136	99.98791	99.98791944	95.0	4.99%	4.99%
52 Acetone	-5.34105	-5.34136	99.98791	99.98791944	96.7	3.29%	3.29%

52 CDCl3	-5.34105	-5.34136	99.98791	99.98791944	97.9	2.09%	2.09%
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.22E4%	1.22E4%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						18.18%	18.18%

Table 1.30: Convergence results from M06 cc-pVDZ gas phase and how it compares to experimental data.

1.7 M06-2X gas phase

1.7.1 M06-2X 6-311++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-2.96879	-2.96937	99.34001	99.3406652	41.7	58.02%	58.02%
2 ethanol	-47191.2	-47191.2	N/A	N/A	44.1	N/A	N/A
3 ethanol	-2.54053	-2.54079	98.64909	98.6496625	44.1	55.30%	55.30%
4 ethanol	-2.55156	-2.55145	98.67368	98.6734538	48.3	51.05%	51.05%
5 ethanol	-2.87957	-2.87964	99.2335	99.23359737	47.6	52.03%	52.03%
6	14.14199	14.14155	4.24E-09	4.23881E-09	6E-7	14065.42%	14054.92%
7	13.8693	13.86921	6.71E-09	6.71434E-09	1.1E-6	16285.28%	16282.86%
8	13.47808	13.47765	1.3E-08	1.30081E-08	1E-6	7593.07%	7587.50%
9	11.1206	11.12072	6.97E-07	6.96638E-07	4E-5	5640.70%	5641.86%
10	9.191128	9.191132	1.81E-05	1.81281E-05	5.5E-4	2933.94%	2933.96%
11	6.610422	6.610813	0.001417	0.001415785	1.4E-2	888.20%	888.85%
12	29.47385	29.47412	2.4E-20	2.40373E-20	0	0.00%	0.00%
13 CDCl3	-3.51023	-3.51092	99.73447	99.73477877	86.0	13.77%	13.77%
13 DMSO	-3.51023	-3.51092	99.73447	99.73477877	63.0	36.83%	36.83%
13	-3.51023	-3.51092	99.73447	99.73477877	80.0	19.79%	19.79%
14 CDCl3	N/A	N/A	N/A	N/A	3.0	N/A	N/A

14 DMSO	N/A	N/A	N/A	N/A	0	N/A	N/A
14	N/A	N/A	N/A	N/A	8.0	N/A	N/A
15 CDCl3	N/A	N/A	N/A	N/A	85.0	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99.0	N/A	N/A
15	N/A	N/A	N/A	N/A	89.0	N/A	N/A
16	-1.2101	-1.20984	88.53175	88.52726546	80.0	9.64%	9.63%
17	-2.7861	-2.78614	99.1036	99.1036679	91.7	7.47%	7.47%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-3.46074	-3.46009	99.71139	99.71107354	95.8	3.92%	3.92%
20	6.145038	6.145828	0.003109	0.003104943	95.3	3065105.74%	3069199.37%
21	-3.73665	-3.73682	99.8187	99.81875134	98.0	1.82%	1.82%
22	-1.87329	-1.87312	95.94514	95.94400764	82.1	14.43%	14.43%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-3.87257	-3.87236	99.85583	99.85578299	93.4	6.47%	6.47%
25	N/A	N/A	N/A	N/A	91.6	N/A	N/A
26	-3.65963	-3.66026	99.79357	99.79378526	93.7	6.11%	6.11%
27	-2.63968	-2.63993	98.855	98.85547832	85.2	13.81%	13.81%
28	-2.22086	-2.22138	97.70426	97.70623483	88.5	9.42%	9.42%
29	-2.75403	-2.75414	99.05418	99.05435783	89.2	9.95%	9.95%
30	-2.80888	-2.80936	99.13714	99.13783876	90.8	8.41%	8.41%

31	-3.54192	-3.54166	99.74827	99.74816673	93.4	6.36%	6.36%
32	-2.31996	-2.32053	98.05118	98.05300806	93.7	4.44%	4.44%
33	-3.34402	-3.344	99.64872	99.64870945	94.6	5.07%	5.07%
34	-2.4487	-2.44854	98.42601	98.42559953	93.9	4.60%	4.60%
35	-2.57981	-2.57969	98.73471	98.73445264	95.9	2.87%	2.87%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	N/A	N/A	N/A	N/A	40.5	N/A	N/A
42 CDCl3	-3.50556	-3.50527	99.73238	99.73224369	92.6	7.15%	7.15%
43 DMSO	-4.72106	-4.72138	99.96557	99.96558547	94.0	5.97%	5.97%
43 Acetone	-4.72106	-4.72138	99.96557	99.96558547	97.7	2.27%	2.27%
43 CDCl3	-4.72106	-4.72138	99.96557	99.96558547	97.8	2.17%	2.17%
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-3.74372	-3.74372	99.82085	99.82084831	94.6	5.23%	5.23%
45Acetone	-3.74372	-3.74372	99.82085	99.82084831	99.3	0.52%	0.52%

45 CDCl3	-3.74372	-3.74372	99.82085	99.82084831	97.3	2.53%	2.53%
46 DMSO	-4.66171	-4.66114	99.96194	99.96190112	93.7	6.26%	6.26%
46 Acetone	-4.66171	-4.66114	99.96194	99.96190112	97.3	2.66%	2.66%
46 CDCl3	-4.66171	-4.66114	99.96194	99.96190112	95.7	4.26%	4.26%
47 DMSO	-6.2508	-6.25062	99.9974	99.9973987	70.1	29.90%	29.90%
47 Acetone	-6.2508	-6.25062	99.9974	99.9973987	87.1	12.90%	12.90%
47 CDCl3	-6.2508	-6.25062	99.9974	99.9973987	86.6	13.40%	13.40%
48 DMSO	10.92593	10.9262	9.68E-07	9.67593E-07	90.7	9369542860.65%	9373779319.33 %
48 Acetone	10.92593	10.9262	9.68E-07	9.67593E-07	95.3	9844734675.63%	9849185993.30 %
48 CDCl3	10.92593	10.9262	9.68E-07	9.67593E-07	95.2	9834404418.79%	9838851065.61 %
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92.0	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-4.23741	-4.23757	99.9221	99.92212019	94.6	5.33%	5.33%
50 Acetone	-4.23741	-4.23757	99.9221	99.92212019	97.8	2.12%	2.12%
50 CDCl3	-4.23741	-4.23757	99.9221	99.92212019	97.2	2.72%	2.72%
51 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A

51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A
51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	-4.23446	-4.23506	99.92171	99.92178959	95.0	4.93%	4.93%
52 Acetone	-4.23446	-4.23506	99.92171	99.92178959	96.7	3.22%	3.22%
52 CDCl3	-4.23446	-4.23506	99.92171	99.92178959	97.9	2.02%	2.02%
Mean Error of Theoretical Calculation of Gas Phase vs literature						5.48E6%	5.48E6%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						12.03%	12.03%

Table 1.31: Convergence results from M06-2X 6-311++G gas phase and how it compares to experimental data.

1.7.2 M06-2X 6-31++G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-2.95927	-2.95933	99.32939	99.32946503	41.7	58.02%	58.02%
2 ethanol	-47177.2	-47177.2	N/A	N/A	44.1	N/A	N/A
3 ethanol	N/A	N/A	N/A	N/A	44.1	N/A	N/A
4 ethanol	-2.68954	-2.68951	98.9465	98.94643409	48.3	51.19%	51.19%
5 ethanol	-2.87343	-2.87337	99.22558	99.22549491	47.6	52.03%	52.03%
6	14.54534	14.54504	2.14E-09	2.14431E-09	6E-7	27895.07%	27881.07%
7	14.15334	14.15285	4.16E-09	4.15871E-09	1.1E-6	26372.58%	26350.50%
8	13.70667	13.70606	8.84E-09	8.84453E-09	1E-6	11218.13%	11206.43%
9	11.213	11.21234	5.96E-07	5.9677E-07	4E-5	6610.27%	6602.75%
10	9.366172	9.366207	1.35E-05	1.34876E-05	5.5E-4	3977.56%	3977.81%
11	6.620671	6.620853	0.001392	0.00139198	1.4E-2	905.45%	905.76%
12	29.68985	29.68998	1.67E-20	1.66936E-20	0	0%	0%
13 CDCl3	N/A	N/A	N/A	N/A	86.0	N/A	N/A
13 DMSO	N/A	N/A	N/A	N/A	63.0	N/A	N/A
13	N/A	N/A	N/A	N/A	80.0	N/A	N/A
14 CDCl3	-1.94767	-1.94779	96.40666	96.40733573	3.0	96.89%	96.89%
14 DMSO	-1.94767	-1.94779	96.40666	96.40733573	0	0%	0%

14	-1.94767	-1.94779	96.40666	96.40733573	8.0	91.70%	91.70%
15 CDCl3	-3.54265	-3.54229	99.74858	99.74843282	85.0	14.79%	14.79%
15 DMSO	-3.54265	-3.54229	99.74858	99.74843282	99.0	0.75%	0.75%
15	-3.54265	-3.54229	99.74858	99.74843282	89.0	10.78%	10.78%
16	-3.01543	-3.01518	99.38971	99.38945291	80.0	19.51%	19.51%
17	-4.35461	-4.35429	99.93608	99.93604503	91.7	8.24%	8.24%
18	-5.74705	-5.74736	99.99391	99.99391423	91.7	8.29%	8.29%
19	-5.55808	-5.55785	99.99162	99.99161876	95.8	4.19%	4.19%
20	6.792242	6.79279	0.001042	0.001041164	95.3	9144650.45%	9153117.07%
21	-4.796	-4.79606	99.96966	99.96966201	98.0	1.97%	1.97%
22	-3.62896	-3.62951	99.78261	99.78281719	82.1	17.72%	17.72%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-5.06562	-5.06526	99.98076	99.98074352	93.4	6.58%	6.58%
25	6.526894	6.527354	0.001631	0.001630095	91.6	5614845.28%	5619204.78%
26	-4.71039	-4.71009	99.96494	99.96492289	93.7	6.27%	6.27%
27	-4.20254	-4.20243	99.91738	99.91736203	85.2	14.73%	14.73%
28	-3.34505	-3.34463	99.64933	99.64908025	88.5	11.19%	11.19%
29	N/A	N/A	N/A	N/A	89.2	N/A	N/A
30	-4.14839	-4.14847	99.90947	99.90948324	90.8	9.12%	9.12%
31	-4.53245	-4.53313	99.95266	99.95271011	93.4	6.56%	6.56%

32	-3.29941	-3.30007	99.62134	99.62175931	93.7	5.94%	5.94%
33	-4.1425	-4.14282	99.90857	99.90861651	94.6	5.31%	5.31%
34	-3.83063	-3.82969	99.84527	99.84502259	93.9	5.95%	5.95%
35	-4.11186	-4.11144	99.90372	99.90364819	95.9	4.01%	4.01%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-2.54364	-2.5433	98.65607	98.65529804	40.5	58.95%	58.95%
42 CDCl3	-4.85063	-4.85065	99.97233	99.97233348	92.6	7.37%	7.37%
43 DMSO	-4.72106	-4.72138	99.96557	99.96558547	94.0	5.97%	5.97%
43 Acetone	-4.72106	-4.72138	99.96557	99.96558547	97.7	2.27%	2.27%
43 CDCl3	-4.72106	-4.72138	99.96557	99.96558547	97.8	2.17%	2.17%
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-3.74372	-3.74372	99.82085	99.82084831	94.6	5.23%	5.23%
45Acetone	-3.74372	-3.74372	99.82085	99.82084831	99.3	0.52%	0.52%
45 CDCl3	-3.74372	-3.74372	99.82085	99.82084831	97.3	2.53%	2.53%

46 DMSO	-4.66171	-4.66114	99.96194	99.96190112	93.7	6.26%	6.26%
46 Acetone	-4.66171	-4.66114	99.96194	99.96190112	97.3	2.66%	2.66%
46 CDCl3	-4.66171	-4.66114	99.96194	99.96190112	95.7	4.26%	4.26%
47 DMSO	-6.2508	-6.25062	99.9974	99.9973987	70.1	29.90%	29.90%
47 Acetone	-6.2508	-6.25062	99.9974	99.9973987	87.1	12.90%	12.90%
47 CDCl3	-6.2508	-6.25062	99.9974	99.9973987	86.6	13.40%	13.40%
48 DMSO	10.92593	10.9262	9.68E-07	9.67593E-07	90.7	9369542860.65%	9373779319.33 %
48 Acetone	10.92593	10.9262	9.68E-07	9.67593E-07	95.3	9844734675.63%	9849185993.30 %
48 CDCl3	10.92593	10.9262	9.68E-07	9.67593E-07	95.2	9834404418.79%	9838851065.61 %
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92.0	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-4.23741	-4.23757	99.9221	99.92212019	94.6	5.33%	5.33%
50 Acetone	-4.23741	-4.23757	99.9221	99.92212019	97.8	2.12%	2.12%
50 CDCl3	-4.23741	-4.23757	99.9221	99.92212019	97.2	2.72%	2.72%
51 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A

51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	-4.23446	-4.23506	99.92171	99.92178959	95.0	4.93%	4.93%
52 Acetone	-4.23446	-4.23506	99.92171	99.92178959	96.7	3.22%	3.22%
52 CDCl3	-4.23446	-4.23506	99.92171	99.92178959	97.9	2.02%	2.02%
Mean Error of Theoretical Calculation of Gas Phase vs literature						5.10E6%	5.10E6%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.92%	14.92%

Table 1.32: Convergence results from M06-2X 6-31++G gas phase and how it compares to experimental data.

1.7.3 M06-2X 6-31+G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-2.9502	-2.95118	99.31912	99.32022591	41.7	58.01%	58.01%
2 ethanol	-47178.4	-47178.4	N/A	N/A	44.1	N/A	N/A
3 ethanol	-3.33714	-3.3371	99.64463	99.64460476	44.1	55.74%	55.74%
4 ethanol	-2.67552	-2.67633	98.92152	98.92297814	48.3	51.17%	51.17%
5 ethanol	N/A	N/A	N/A	N/A	47.6	N/A	N/A
6	14.66468	14.6649	1.75E-09	1.75136E-09	6E-7	34146.61%	34159.17%
7	14.19579	14.19552	3.87E-09	3.86955E-09	1.1E-6	28340.18%	28327.10%
8	13.81242	13.81211	7.39E-09	7.39415E-09	1E-6	13431.14%	13424.21%
9	11.28733	11.28764	5.26E-07	5.25502E-07	4E-5	7507.79%	7511.77%
10	9.448282	9.447783	1.17E-05	1.17517E-05	5.5E-4	4584.12%	4580.18%
11	6.690401	6.690506	0.001238	0.001237494	1.4E-2	1031.12%	1031.32%
12	29.77168	29.77219	1.45E-20	1.45296E-20	0	0.00%	0.00%
13 CDCl3	-4.5392	-4.53878	99.95319	99.95315882	86.0	13.96%	13.96%
13 DMSO	-4.5392	-4.53878	99.95319	99.95315882	63.0	36.97%	36.97%
13	-4.5392	-4.53878	99.95319	99.95315882	80.0	19.96%	19.96%
14 CDCl3	-1.91183	-1.91202	96.19094	96.19213292	3.0	96.88%	96.88%
14 DMSO	-1.91183	-1.91202	96.19094	96.19213292	0	0.00%	0.00%

14	-1.91183	-1.91202	96.19094	96.19213292	8.0	91.68%	91.68%
15 CDCl3	-3.49782	-3.49837	99.72886	99.72911241	85.0	14.77%	14.77%
15 DMSO	-3.49782	-3.49837	99.72886	99.72911241	99.0	0.73%	0.73%
15	-3.49782	-3.49837	99.72886	99.72911241	89.0	10.76%	10.76%
16	N/A	N/A	N/A	N/A	80.0	N/A	N/A
17	-4.89038	-4.89018	99.97413	99.97411996	91.7	8.28%	8.28%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-5.58177	-5.5817	99.99195	99.99194956	95.8	4.19%	4.19%
20	6.432827	6.4326	0.001912	0.001912992	95.3	4983535.11%	4981624.73%
21	-4.77977	-4.77974	99.96882	99.96881468	98.0	1.97%	1.97%
22	-3.5952	-3.595	99.76989	99.76981132	82.1	17.71%	17.71%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-5.04029	-5.04016	99.97991	99.9799098	93.4	6.58%	6.58%
25	6.640746	6.640933	0.001346	0.001345564	91.6	6805309.06%	6807454.37%
26	-4.66917	-4.6693	99.96241	99.96242224	93.7	6.26%	6.26%
27	-4.16594	-4.16604	99.91211	99.91212753	85.2	14.73%	14.73%
28	-3.31614	-3.31639	99.63185	99.63200176	88.5	11.17%	11.17%
29	-4.50447	-4.50426	99.95037	99.95034869	89.2	10.76%	10.76%
30	-4.11463	-4.11458	99.90416	99.90415693	90.8	9.11%	9.11%
31	N/A	N/A	N/A	N/A	93.4	N/A	N/A

32	-3.24964	-3.24924	99.58827	99.58799424	93.7	5.91%	5.91%
33	-4.02013	-4.01983	99.8876	99.88754209	94.6	5.29%	5.29%
34	N/A	N/A	N/A	N/A	93.9	N/A	N/A
35	-2.21719	-2.21699	97.69029	97.6895493	95.9	1.83%	1.83%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-2.60924	-2.60918	98.79533	98.79520646	40.5	59.01%	59.01%
42 CDCl3	-4.82588	-4.82618	99.97115	99.97116632	92.6	7.37%	7.37%
43 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
43 Acetone	N/A	N/A	N/A	N/A	97.7	N/A	N/A
43 CDCl3	N/A	N/A	N/A	N/A	97.8	N/A	N/A
44 DMSO	N/A	N/A	N/A	N/A	90.2	N/A	N/A
44 Acetone	N/A	N/A	N/A	N/A	93.6	N/A	N/A
44 CDCl3	N/A	N/A	N/A	N/A	91.6	N/A	N/A
45 DMSO	-3.98191	-3.98218	99.88011	99.88016755	94.6	5.29%	5.29%
45Acetone	-3.98191	-3.98218	99.88011	99.88016755	99.3	0.58%	0.58%
45 CDCl3	-3.98191	-3.98218	99.88011	99.88016755	97.3	2.58%	2.58%

46 DMSO	-4.67806	-4.67808	99.96297	99.96297548	93.7	6.27%	6.27%
46 Acetone	-4.67806	-4.67808	99.96297	99.96297548	97.3	2.66%	2.66%
46 CDCl3	-4.67806	-4.67808	99.96297	99.96297548	95.7	4.26%	4.26%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	11.39577	11.39495	4.38E-07	4.38397E-07	90.7	20718027313.26%	20689029232.16%
48 Acetone	11.39577	11.39495	4.38E-07	4.38397E-07	95.3	21768776222.87%	21738307456.28%
48 CDCl3	11.39577	11.39495	4.38E-07	4.38397E-07	95.2	21745933855.27%	21715497060.10%
49 DMSO	-5.53675	-5.53714	99.99131	99.99132047	82.5	17.49%	17.49%
49 Acetone	-5.53675	-5.53714	99.99131	99.99132047	92.0	7.99%	7.99%
49 CDCl3	-5.53675	-5.53714	99.99131	99.99132047	88.2	11.79%	11.79%
50 DMSO	-4.31393	-4.31413	99.93154	99.93155962	94.6	5.34%	5.34%
50 Acetone	-4.31393	-4.31413	99.93154	99.93155962	97.8	2.13%	2.13%
50 CDCl3	-4.31393	-4.31413	99.93154	99.93155962	97.2	2.73%	2.73%
51 DMSO	N/A	N/A	N/A	N/A	94.0	N/A	N/A
51 Acetone	N/A	N/A	N/A	N/A	96.4	N/A	N/A

51 CDCl3	N/A	N/A	N/A	N/A	96.1	N/A	N/A
52 DMSO	N/A	N/A	N/A	N/A	95.0	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A
52 CDCl3	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.26E7%	1.26E7%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						17.25%	17.25%

Table 1.33: Convergence results from M06-2X 6-31+G gas phase and how it compares to experimental data.

1.7.4 M06-2X 6-31G

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-3.12445	-3.12437	99.49182	99.49174918	41.7	58.09%	58.09%
2 ethanol	-47175.9	-47175.9	N/A	N/A	44.1	N/A	N/A
3 ethanol	-3.50355	-3.50339	99.73147	99.7313933	44.1	55.78%	55.78%
4 ethanol	-2.65176	-2.65248	98.87786	98.87921376	48.3	51.15%	51.15%
5 ethanol	-3.02886	-3.02899	99.40331	99.40343987	47.6	52.11%	52.11%
6	16.03757	16.03663	1.72E-10	1.72669E-10	6E-7	347938.30%	347386.46%
7	15.57313	15.5729	3.78E-10	3.77882E-10	1.1E-6	291107.26%	290995.93%
8	14.58855	14.58897	1.99E-09	1.99098E-09	1E-6	50091.01%	50126.43%
9	11.95209	11.95217	1.71E-07	1.71058E-07	4E-5	23280.65%	23283.90%
10	N/A	N/A	N/A	N/A	5.5E-4	N/A	N/A
11	8.303827	8.303833	8.11E-05	8.113E-05	1.4E-2	17156.09%	17156.27%
12	30.93542	30.93559	2.04E-21	2.0366E-21	0	0.00%	0.00%
13 CDCl3	N/A	N/A	N/A	N/A	86.0	N/A	N/A
13 DMSO	N/A	N/A	N/A	N/A	63.0	N/A	N/A
13	N/A	N/A	N/A	N/A	80.0	N/A	N/A
14 CDCl3	-1.83066	-1.83107	95.65558	95.65848608	3.0	96.86%	96.86%
14 DMSO	-1.83066	-1.83107	95.65558	95.65848608	0	0.00%	0.00%

14	-1.83066	-1.83107	95.65558	95.65848608	8.0	91.64%	91.64%
15 CDCl3	N/A	N/A	N/A	N/A	85.0	N/A	N/A
15 DMSO	N/A	N/A	N/A	N/A	99.0	N/A	N/A
15	N/A	N/A	N/A	N/A	89.0	N/A	N/A
16	-2.54353	-2.5433	98.65581	98.65529804	80.0	18.91%	18.91%
17	-5.11553	-5.11546	99.98231	99.98230862	91.7	8.28%	8.28%
18	N/A	N/A	N/A	N/A	91.7	N/A	N/A
19	-4.53462	-4.53438	99.95283	99.95281019	95.8	4.15%	4.15%
20	N/A	N/A	N/A	N/A	95.3	N/A	N/A
21	-4.26431	-4.26455	99.92556	99.92558711	98.0	1.93%	1.93%
22	-3.62371	-3.62387	99.78068	99.78074027	82.1	17.72%	17.72%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-5.01037	-5.01004	99.97887	99.97886156	93.4	6.58%	6.58%
25	7.312777	7.312368	0.000433	0.000432926	91.6	21172849.37%	21158228.33%
26	-4.48451	-4.48418	99.94867	99.9486368	93.7	6.25%	6.25%
27	-4.22863	-4.22879	99.92094	99.92095695	85.2	14.73%	14.73%
28	-2.68514	-2.68574	98.93873	98.93978445	88.5	10.55%	10.55%
29	N/A	N/A	N/A	N/A	89.2	N/A	N/A
30	-3.05554	-3.05534	99.42945	99.42926371	90.8	8.68%	8.68%
31	-4.43295	-4.43273	99.944	99.94397597	93.4	6.55%	6.55%

32	-3.31487	-3.31513	99.63106	99.63122379	93.7	5.95%	5.95%
33	-4.18021	-4.18047	99.9142	99.9142418	94.6	5.32%	5.32%
34	N/A	N/A	N/A	N/A	93.9	N/A	N/A
35	-3.8562	-3.85667	99.8518	99.85191654	95.9	3.96%	3.96%
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	N/A	N/A	N/A	N/A	40.5	N/A	N/A
42 CDCl3	-5.09459	-5.09538	99.98167	99.98169845	92.6	7.38%	7.38%
43 DMSO	-4.17983	-4.17921	99.91415	99.91405998	94.0	5.92%	5.92%
43 Acetone	-4.17983	-4.17921	99.91415	99.91405998	97.7	2.22%	2.22%
43 CDCl3	-4.17983	-4.17921	99.91415	99.91405998	97.8	2.12%	2.12%
44 DMSO	-5.42172	-5.42168	99.98945	99.98945179	90.2	9.79%	9.79%
44 Acetone	-5.42172	-5.42168	99.98945	99.98945179	93.6	6.39%	6.39%
44 CDCl3	-5.42172	-5.42168	99.98945	99.98945179	91.6	8.39%	8.39%
45 DMSO	-4.9077	-4.90775	99.97487	99.97487648	94.6	5.38%	5.38%
45Acetone	-4.9077	-4.90775	99.97487	99.97487648	99.3	0.68%	0.68%
45 CDCl3	-4.9077	-4.90775	99.97487	99.97487648	97.3	2.68%	2.68%

46 DMSO	-4.2072	-4.20682	99.91802	99.91797234	93.7	6.22%	6.22%
46 Acetone	-4.2072	-4.20682	99.91802	99.91797234	97.3	2.62%	2.62%
46 CDCl3	-4.2072	-4.20682	99.91802	99.91797234	95.7	4.22%	4.22%
47 DMSO	-5.80797	-5.8076	99.99451	99.99450293	70.1	29.90%	29.90%
47 Acetone	-5.80797	-5.8076	99.99451	99.99450293	87.1	12.90%	12.90%
47 CDCl3	-5.80797	-5.8076	99.99451	99.99450293	86.6	13.40%	13.40%
48 DMSO	N/A	N/A	N/A	N/A	90.7	N/A	N/A
48 Acetone	N/A	N/A	N/A	N/A	95.3	N/A	N/A
48 CDCl3	N/A	N/A	N/A	N/A	95.2	N/A	N/A
49 DMSO	N/A	N/A	N/A	N/A	82.5	N/A	N/A
49 Acetone	N/A	N/A	N/A	N/A	92.0	N/A	N/A
49 CDCl3	N/A	N/A	N/A	N/A	88.2	N/A	N/A
50 DMSO	-4.00451	-4.00414	99.8846	99.88452612	94.6	5.29%	5.29%
50 Acetone	-4.00451	-4.00414	99.8846	99.88452612	97.8	2.09%	2.09%
50 CDCl3	-4.00451	-4.00414	99.8846	99.88452612	97.2	2.69%	2.69%
51 DMSO	-4.02333	-4.02296	99.8882	99.88813578	94.0	5.89%	5.89%
51 Acetone	-4.02333	-4.02296	99.8882	99.88813578	96.4	3.49%	3.49%
51 CDCl3	-4.02333	-4.02296	99.8882	99.88813578	96.1	3.79%	3.79%
52 DMSO	-3.89581	-3.89621	99.86137	99.86146779	95.0	4.87%	4.87%
52 Acetone	-3.89581	-3.89621	99.86137	99.86146779	96.7	3.17%	3.17%

52 CDCl3	-3.89581	-3.89621	99.86137	99.86146779	97.9	1.96%	1.96%
Mean Error of Theoretical Calculation of Gas Phase vs literature						4.13E3%	4.13E3%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						14.44%	14.44%

Table 1.34: Convergence results from M06-2X 6-31G gas phase and how it compares to experimental data.

1.7.5 M06-2X cc-pVDZ

CPD No.	ΔG Calculated	ΔG Programme	Enol% Calculated	Enol% Programme	Experimental enol%	Error Calc.	Error Prog.
1 ethanol	-3.35335	-3.35341	99.6542	99.65423072	41.7	58.16%	58.16%
2 ethanol	-47181.3	-47181.3	N/A	N/A	44.1	N/A	N/A
3 ethanol	-2.54884	-2.54957	98.66766	98.66928559	44.1	55.30%	55.31%
4 ethanol	-2.64814	-2.64872	98.87106	98.87214469	48.3	51.15%	51.15%
5 ethanol	-3.03839	-3.0384	99.41279	99.41279335	47.6	52.12%	52.12%
6	14.9891	14.98932	1.01E-09	1.01254E-09	6E-7	59134.64%	59156.91%
7	14.64718	14.6467	1.8E-09	1.80602E-09	1.1E-6	60857.25%	60807.43%
8	13.50599	13.50651	1.24E-08	1.23892E-08	1E-6	7964.37%	7971.57%
9	11.23934	11.23932	5.7E-07	5.70184E-07	4E-5	6915.43%	6915.27%
10	9.869358	9.869469	5.77E-06	5.76495E-06	5.5E-4	9438.61%	9440.41%
11	7.856753	7.857046	0.000173	0.000172543	1.4E-2	8009.91%	8013.93%
12	29.57698	29.57703	2.02E-20	2.02023E-20	0	0%	0%
13 CDCl3	-4.7864	-4.78664	99.96916	99.96917601	86.0	13.97%	13.97%
13 DMSO	-4.7864	-4.78664	99.96916	99.96917601	63.0	36.98%	36.98%
13	-4.7864	-4.78664	99.96916	99.96917601	80.0	19.98%	19.98%
14 CDCl3	-2.54974	-2.54957	98.66967	98.66928559	3.0	96.96%	96.96%
14 DMSO	-2.54974	-2.54957	98.66967	98.66928559	0	0%	0%

14	-2.54974	-2.54957	98.66967	98.66928559	8.0	91.89%	91.89%
15 CDCl3	-4.77296	-4.77346	99.96846	99.96848252	85.0	14.97%	14.97%
15 DMSO	-4.77296	-4.77346	99.96846	99.96848252	99.0	0.97%	0.97%
15	-4.77296	-4.77346	99.96846	99.96848252	89.0	10.97%	10.97%
16	-2.8514	-2.85203	99.19645	99.19730561	80.0	19.35%	19.35%
17	-5.68837	-5.68775	99.99328	99.99326963	91.7	8.29%	8.29%
18	-6.09938	-6.10002	99.99664	99.99664531	91.7	8.30%	8.30%
19	-5.15439	-5.15436	99.98343	99.98343354	95.8	4.18%	4.18%
20	7.670094	7.670049	0.000237	0.000236624	95.3	40277884.91%	40274816.47%
21	-4.60717	-4.60717	99.95827	99.95826696	98.0	1.96%	1.96%
22	-4.11734	-4.11709	99.9046	99.90456199	82.1	17.82%	17.82%
23	N/A	N/A	N/A	N/A	91.6	N/A	N/A
24	-5.61202	-5.61119	99.99235	99.99234072	93.4	6.59%	6.59%
25	7.460118	7.459205	0.000337	0.000337839	91.6	27155222.75%	27113380.94%
26	-5.16776	-5.16754	99.9838	99.98379812	93.7	6.28%	6.28%
27	-4.72163	-4.72138	99.9656	99.96558547	85.2	14.77%	14.77%
28	-3.21114	-3.21097	99.56073	99.56059947	88.5	11.11%	11.11%
29	-3.91342	-3.91315	99.86543	99.86537047	89.2	10.68%	10.68%
30	-5.3006	-5.30057	99.98706	99.987058	90.8	9.19%	9.19%
31	-5.09701	-5.09726	99.98175	99.98175653	93.4	6.58%	6.58%

32	-3.6754	-3.67595	99.79898	99.79916646	93.7	6.11%	6.11%
33	N/A	N/A	N/A	N/A	94.6	N/A	N/A
34	-4.48496	-4.48481	99.9487	99.94869118	93.9	6.05%	6.05%
35	N/A	N/A	N/A	N/A	95.9	N/A	N/A
36	N/A	N/A	N/A	N/A	95.6	N/A	N/A
37	N/A	N/A	N/A	N/A	97.0	N/A	N/A
38	N/A	N/A	N/A	N/A	97.4	N/A	N/A
39	N/A	N/A	N/A	N/A	96.8	N/A	N/A
40	N/A	N/A	N/A	N/A	98.1	N/A	N/A
41 CDCl3	-3.01361	-3.0133	99.38784	99.38752052	40.5	59.25%	59.25%
42 CDCl3	-5.59888	-5.59864	99.99218	99.99217665	92.6	7.39%	7.39%
43 DMSO	-5.13281	-5.13303	99.98282	99.98282581	94.0	5.98%	5.98%
43 Acetone	-5.13281	-5.13303	99.98282	99.98282581	97.7	2.28%	2.28%
43 CDCl3	-5.13281	-5.13303	99.98282	99.98282581	97.8	2.18%	2.18%
44 DMSO	-6.04168	-6.04166	99.9963	99.99629783	90.2	9.80%	9.80%
44 Acetone	-6.04168	-6.04166	99.9963	99.99629783	93.6	6.40%	6.40%
44 CDCl3	-6.04168	-6.04166	99.9963	99.99629783	91.6	8.40%	8.40%
45 DMSO	-5.32132	-5.32128	99.9875	99.98750276	94.6	5.39%	5.39%
45Acetone	-5.32132	-5.32128	99.9875	99.98750276	99.3	0.69%	0.69%
45 CDCl3	-5.32132	-5.32128	99.9875	99.98750276	97.3	2.69%	2.69%

46 DMSO	-5.28131	-5.28049	99.98663	99.98661162	93.7	6.29%	6.29%
46 Acetone	-5.28131	-5.28049	99.98663	99.98661162	97.3	2.69%	2.69%
46 CDCl3	-5.28131	-5.28049	99.98663	99.98661162	95.7	4.29%	4.29%
47 DMSO	N/A	N/A	N/A	N/A	70.1	N/A	N/A
47 Acetone	N/A	N/A	N/A	N/A	87.1	N/A	N/A
47 CDCl3	N/A	N/A	N/A	N/A	86.6	N/A	N/A
48 DMSO	-4.89292	-4.89332	99.97424	99.97425671	90.7	9.28%	9.28%
48 Acetone	-4.89292	-4.89332	99.97424	99.97425671	95.3	4.68%	4.68%
48 CDCl3	-4.89292	-4.89332	99.97424	99.97425671	95.2	4.78%	4.78%
49 DMSO	-6.27535	-6.27572	99.99751	99.99750667	82.5	17.50%	17.50%
49 Acetone	-6.27535	-6.27572	99.99751	99.99750667	92.0	8.00%	8.00%
49 CDCl3	-6.27535	-6.27572	99.99751	99.99750667	88.2	11.80%	11.80%
50 DMSO	-5.03383	-5.03388	99.97969	99.97969579	94.6	5.38%	5.38%
50 Acetone	-5.03383	-5.03388	99.97969	99.97969579	97.8	2.18%	2.18%
50 CDCl3	-5.03383	-5.03388	99.97969	99.97969579	97.2	2.78%	2.78%
51 DMSO	-5.07036	-5.07028	99.98091	99.98090606	94.0	5.98%	5.98%
51 Acetone	-5.07036	-5.07028	99.98091	99.98090606	96.4	3.58%	3.58%
51 CDCl3	-5.07036	-5.07028	99.98091	99.98090606	96.1	3.88%	3.88%
52 DMSO	N/A	N/A	N/A	N/A	95.0	N/A	N/A
52 Acetone	N/A	N/A	N/A	N/A	96.7	N/A	N/A

52 $CDCl_3$	N/A	N/A	N/A	N/A	97.9	N/A	N/A
Mean Error of Theoretical Calculation of Gas Phase vs literature						1.07E4%	1.07E4%
Mean Error of Theoretical Calculation of Gas Phase vs literature with outliers removed						15.35%	15.35%

Table 1.35: Convergence results from M06-2X cc-pVDZ gas phase and how it compares to experimental data.