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Interaction-Induced Dipole Moments of Carbon Dioxide

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To the Graduate Council:

I am submitting herewith a dissertation written by Randi Lynn Beil entitled "Interaction-Induced Dipole Moments of Carbon Dioxide." I have examined the final electronic copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Chemistry.

Robert J Hinde, Major Professor

We have read this dissertation and recommend its acceptance:

Craig Barnes, Bhavya Sharma, Lucas Platter

Accepted for the Council:

Dixie L. Thompson

Vice Provost and Dean of the Graduate School

(Original signatures are on file with official student records.)

Interaction-Induced Dipole Moments of Carbon Dioxide

A Dissertation Presented for the

Doctor of Philosophy

Degree

The University of Tennessee, Knoxville

Randi Lynn Beil

August 2019

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To my family

Acknowledgments

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Abstract

The atmospheric absorption spectrum of carbon dioxide-rich planetary atmospheres, such as Venus or ancient Mars, can be difficult to model due to the presence of collision-induced absorption (CIA) features. These features appear in the 0-250 cm^{-1} range and are caused by the interaction-induced (I-I) dipole moments of a carbon dioxide dimer. Studying these I-I dipole moments can lead to more accurate atmospheric models, which can be used to create better estimates of the surface temperature of these planets and can reveal information about their paleoclimates. The GAMESS *ab initio* software package and the NWChem *ab initio* software package were used with a finite-field approach to calculate the polarizabilities, hyperpolarizabilities, quadrupole moment, and hexadecapole moment for a carbon dioxide monomer. The basis set and bond length dependence of these values were investigated at the Hartree-Fock, MP2, CCSD, and CCSD(T) levels of theory. The energies and dipole moments of a T-shaped CO_2 dimer as a function of the intermolecular distance were also calculated. These calculations were performed using the aug-cc-pVTZ, aug-cc-pVQZ, and aug-pc-3 basis sets. Using the monomer results as fitting parameters, a function modeling the counterpoise-corrected dipole moments was developed and compared to an equation developed analytically by M. S. A. El-Kader and G. Maroulis.

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Chapter 1

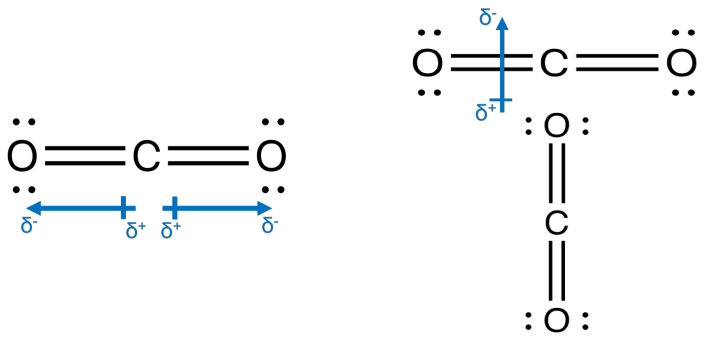
Introduction

The planet Mars has been the subject of much scientific interest and exploration. Images from the surface of the planet have shown it to be dusty, rocky, and dry; temperatures on the planet average around -63 °C [24], and liquid water, if present, is scarce. Despite the current lack of water, certain formations found on the planet, such as dried river deltas, are thought to have been caused by flowing water [6]. The evidence of liquid water on Mars raises many questions about its paleoclimate: for liquid water to have once existed, the planet must have been warm enough where water could be in its liquid state. However, almost 3.5 billion years ago when the rivers and lakes were thought to have been present on Mars, the sun was not as bright as it is now [12, 38]. It would not have been possible for the sun to warm the planet enough for liquid water to have existed. Many theories attempting to explain this issue, known as the early warming problem, rely on a thick, carbon dioxide-rich atmosphere [38].

The current atmosphere of Mars is approximately 95% carbon dioxide and has an average pressure of 6.27×10^{-3} atm [36]. The atmosphere is thin, and most of its gases have been blown away by solar winds [25]. The ancient atmosphere is also thought to have been mostly carbon dioxide at pressures of least 0.5 atm [18], but the exact pressure and composition is still an active area of research. Accurately modeling the atmosphere of Mars is important for surface temperature calculations, but optical properties of a dense atmosphere are difficult to model correctly due to the presence of collision-induced absorptions (CIA) [38].

Collision-induced absorptions occur when two molecules, CO_2 in the case of the Martian atmosphere, approach each other and induce a dipole in one another. Carbon dioxide does not have a dipole moment, but it does have a quadrupole moment (Figure 1.1a). When two molecules are close, the quadrupole moments on the molecules can interact and induce a dipole moment in one another (Figure 1.1b). These interaction-induced dipole moments appear in the 0-250 cm^{-1} region of the infrared spectrum [38]. Models describing these interactions exist, but many were parameterized using data from Venus, which has a thicker and hotter atmosphere than what Mars ever did [38]. Furthermore, these models do not agree with one another; this can be seen in Figure 2 of Reference [38]. Because these models give different results, and experimental data of the ancient Martian atmosphere does not exist to give better parameters, the most accurate model can not be easily determined.

In order to find a reliable and accurate atmospheric model, we will use *ab initio* methods to develop a model for the collision-induced absorptions that is independent of any experimental variables. This will ensure that the created model is not relying on external parameters and can be used to compare existing models. Before modeling CIA, the polarizability and hyperpolarizability of CO_2 must be calculated to a high degree of accuracy, along with the interaction-induced dipole moment of $(CO_2)_2$. The theory and methods used to calculate CIA models are discussed in Chapter 2. The mathematical methods used in this work to calculate the properties of CO_2 and $(CO_2)_2$ are described in Chapter 3, and the results of this work are presented in Chapters 4 and 5.



(a) CO_2 Quadrupole **(b)** $(CO_2)_2$ Dipole

Figure 1.1: Carbon dioxide does not have a dipole moment, but it has a quadrupole moment which can induce a dipole when in a dimer configuration.

Chapter 2

Modeling Collision-Induced Absorptions

As mentioned in Chapter 1, the interaction of two carbon dioxide molecules can create an induced dipole moment. These interaction-induced dipole moments are IR-active and appear in the 0-250 cm^{-1} region. Previous work on these collision-induced absorption models has relied on the use of experimental data, semi-empirical methods, and classical mechanics to compute and correct the models. By modeling CIA with *ab initio* methods, an atmospheric model can be developed that is based solely on quantum mechanical results.

2.1 Methods Used in Modeling CIA

Modeling CIA is usually done by calculating potential energy surfaces (PES) of the CO_2 dimer. The potential energy surfaces, consisting of the energies of the dimer in various configurations, are used in molecular dynamics (MD) simulations. The trajectories of these simulations are then used to calculate the interaction-induced dipole moment [1], and the function describing the time-dependent dipole moments is Fourier transformed to obtain the spectrum [10]. The spectrum is compared to experimental data of dense carbon dioxide gas, and corrections to the function are made to ensure an accurate fit.

2.2 Early Literature Results

The accuracy of these models therefore relies on the accuracy of the PES and the quality of the experimental data. The functions are calibrated to particular sets of experimental data; Pollack *et al.*'s parameterization [27], based on experimental data from Venus, has been used extensively in the development of atmospheric models [38]. One such model, developed by Kasting *et al.* [16], is one of the most commonly used models of CIA [38], but it has been shown to produce inaccurate pressure and temperature calculations [38].

The work of Gruszka and Borysow [9] has also been widely cited in the CIA literature. The results they obtained from MD simulations were compared to experimental data from Venus, and corrections parameterized from this data were included in their fit. Although they were able to obtain good agreement with experimental data after their corrections, these corrections have been shown to be unnecessary when using a different potential energy surface [10].

2.3 Modern Literature Results

There have been numerous efforts to achieve a better description of the collision-induced absorptions using more robust computational methods. Most of the research has been focused on calculating highly accurate potential energy surfaces to be used in the MD simulations. Because the potential energy surface is used to calculate the trajectories, and the trajectories are used to calculate the induced dipole moments, if the potential energy surface is inaccurate, the calculated dipole moments will consequently also be inaccurate. Hartmann *et al.* [10] demonstrated the difference between different potential energy surfaces in the molecular dynamics calculations; the two potential energy surfaces derived from *ab initio* values performed significantly better in comparison with experiment than the PES not formulated from *ab initio* results.

The induced dipole moments calculated in Reference [10] were determined through the use of a general model, Eq. 2.1, the geometric variables of which are from the trajectories of the classical MD simulation. The MD-calculated induced dipole moments are therefore

calculated from an approximate model. Using *ab initio* results, we can develop an exact model that describes the values. Furthermore, the $A_{l_1,l_2,\Lambda,L}$ term is reliant upon accurate values for the polarizability, quadrupole moment, and hexadecapole moment of a single carbon dioxide molecule; these values can also be accurately calculated using *ab initio* methods.

$$\mu_{1,2}^{ind}(n=0,\pm1) = \frac{(4\pi)^(3/2)}{\sqrt{3}} \sum_{l_1,l_2,\Lambda,L} A_{l_1,l_2,\Lambda,L}(R_{12}) \sum_{m_\Lambda,m,m_1,m_2} (-1)^{l_1+l_2+m_\Lambda+\Lambda+l+n} \sqrt{3(2\Lambda+1)} \times \begin{pmatrix} \Lambda & l & 1 \\ m_\Lambda & m & -n \end{pmatrix} \begin{pmatrix} l_1 & l_2 & \Lambda \\ m_1 & m_2 & -m_\Lambda \end{pmatrix} Y_{l_1,m_1}(\theta_1,\phi_1) Y_{l_2,m_2}(\theta_2,\phi_2) Y_{l,m}(\theta,\phi) \tag{2.1}$$

Kalugina *et al.* [14] calculated the PES using CCSD(T)-F12b with the aug-cc-pVTZ basis set. This high level of computational theory coupled with a relatively large basis set produced a PES thought to be very accurate; they stated that an induced dipole moment surface was calculated, but no work detailing the methods or results has been published. El-Kader and Maroulis [5] attempted to use an equation similar to Eq. 2.1 to obtain an expression to describe the interaction-induced dipole moments in $(CO_2)_2$. However, the final fitting equation was parameterized with values obtained from experimental data and is not solely composed of *ab initio* results. This fitting equation is discussed in Section 3.3 and is compared to *ab initio* results in Section 5.2.2.

Thus, to the best of our knowledge, there has been no reported induced dipole moment model derived from *ab initio* properties. Calculating these models will require high-level calculations of the polarizabilities, quadrupole moment, and hexadecapole moment of a CO_2 monomer, which we have done in Chapter 4. *ab initio* calculations of the dipole moment of $(CO_2)_2$ are also required to provide a high-quality data set to which a model can be fit; the results of this fitting are listed in Chapter 5.

Chapter 3

Calculating the Properties of CO_2 and $(CO_2)_2$

This chapter presents the methods that were used to calculate the values needed to find a model for the interaction-induced dipole moments. The primary technique involves fitting *ab initio* obtained values to a function and deriving the appropriate property from these fits. The methods used for the monomer results are in Section 3.2, and the methods used for the dimer results are in Section 3.3.

3.1 Computational Methods

3.1.1 Levels of Theory

To calculate these properties, first we must consider which computational theory to use. The four methods used in this work are restricted Hartree-Fock (RHF), 2nd order Møller-Plesset perturbation theory (MP2), and coupled cluster using singles and doubles (CCSD) and perturbative triples (CCSD(T)). RHF is used for closed-shell systems and does not include electron correlation. It is the lowest level of theory, and as a result, is also the fastest. RHF also allows for the direct computation of polarizabilities and hyperpolarizabilities. Although it is not as exact as the other methods, we used RHF as a starting point in order

to validate and benchmark the methods we will be using to calculate the polarizabilities and hyperpolarizabilities.

MP2, which is the next highest level of theory, begins with the Hartree-Fock wavefunction, then adds a correction to account for electron correlation. CCSD and CCSD(T) are the highest levels of theory used here, with CCSD(T) being considered "the gold standard." In CC methods, an excitation operator is used in conjunction with the Hartree-Fock wavefunction to account for more electron correlation. CCSD includes single and double excitations, and CCSD(T) adds triple excitations perturbatively [19, 22]. Since CCSD and CCSD(T) calculations are computationally intensive, we will use these methods only after benchmarking and verifying the methods with RHF.

3.1.2 Basis Sets

In addition to the level of theory, we must also consider which basis sets to use. Basis sets are a group of functions that collectively describe the orbitals of a molecule. Including more functions provides a more accurate description of the orbitals and thus leads to more accurate results; however, adding more basis functions also increases the time it takes to perform the calculation. As a result, it is important to choose basis sets that are large enough to be accurate, but not so large that the calculations are too computationally intensive.

The basis sets used in the work are cc-pVNZ and aug-cc-pVNZ where N ranges from D (double) to Q (quadruple), pc-3, aug-pc-3, and aug-pc-4 [28, 30, 17, 4, 13, 7, 37]. Table 3.1 lists the number of each type of orbital included in the basis sets, along with the total number of orbitals for a single CO_2 molecule. The smallest basis sets belong to the cc-pVNZ family. These are the Dunning correlation-consistent basis sets and were designed to be used with coupled-cluster calculations. The aug-cc-pVNZ family, the augmented versions of the cc-pVNZ basis sets, include diffuse functions. These diffuse functions are used to describe the outer edges of the orbitals, and are particularly important for dipole and polarizability calculations. The d-aug-cc-pVNZ family adds an additional set of diffuse functions. The pc-3 and aug-pc-N basis sets were developed for Hartree-Fock and DFT for the calculation of response properties. Although they were not developed with MP2 or coupled-cluster methods in mind, they may provide good results for the polarizabilities and hyperpolarizabilities.

Table 3.1: The basis sets used in this work.

Basis Set	Abbreviation	Number of Orbitals	Total Orbitals (CO_2)
cc-pVDZ	CCD	3s 3p 1d	42
cc-pVTZ	CCT	4s 3p 2d 1f	90
cc-pVQZ	CCQ	5s 4p 3d 2f 1g	165
aug-cc-pVDZ	ACCD	4s 3p 2d	69
aug-cc-pVTZ	ACCT	5s 4p 3d 2f	138
aug-cc-pVQZ	ACCQ	6s 5p 4d 3f 2g	240
d-aug-cc-pVDZ	DACCD	5s 4p 3d	96
d-aug-cc-pVTZ	DACCT	6s 5p 4d 3f	186
pc-3	PC3	6s 5p 4d 2f 1g	192
aug-pc-3	APC3	7s 6p 5d 3f 2g	267
aug-pc-4	APC4	9s 8p 7d 4f 3g 2h	435

3.2 Calculating the Polarizabilities and Hyperpolarizabilities

Accurate polarizabilities are needed as these values are used directly in the function describing the induced dipole moment of $(CO_2)_2$. As the energy is comprised of contributions from both the polarizability and hyperpolarizability (Eq. 3.3), accurate hyperpolarizabilities are required to ensure that the values calculated for the polarizabilities are not contaminated by contributions from higher order terms. The following section discusses the methods used to calculate these values.

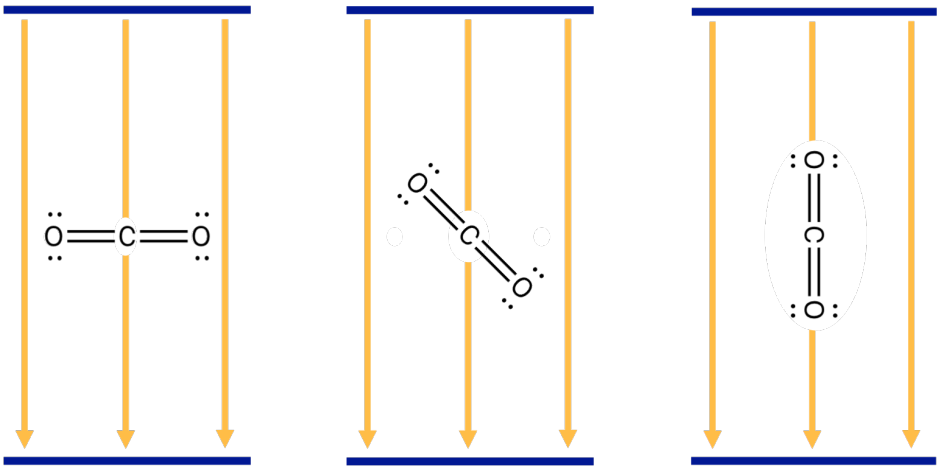
3.2.1 The Finite-Field Method

The finite-field method is a technique used to calculate dipole moments or other field-dependent properties when the level of theory used does not output them directly. In this method, a molecule is placed in an electric field at various field strengths, and the energy is calculated at each field strength. For this work, the electric field is in the x-direction with the molecule perpendicular to the electric field, the z-direction with the molecule parallel to the electric field, and the xz-direction with the molecule at a 45° angle in the electric field (Figure 3.1).

The strength of the field used depends upon which property is to be calculated. The energies are then plotted against the field strengths, and the resulting fit is used to calculate the necessary values. The polarizabilities and hyperpolarizabilities of CO_2 were calculated using the finite-field method, as were the dipole moments of the CO_2 dimer at the CCSD and CCSD(T) levels of theory.

3.2.2 Deriving the Equations used to Solve for the Polarizabilities and Hyperpolarizabilities

Polarizability is the degree to which electrons in a molecule will be disturbed by an electric field, where the polarizability is a second order term with respect to the field, and the hyperpolarizabilities are any higher order terms. The polarizability and hyperpolarizability



(a) X-Direction **(b)** XZ-Direction **(c)** Z-Direction

Figure 3.1: The positions of a carbon dioxide molecule in an electric field.

can be calculated using an equation described by A. D. Buckingham [3]. The full equation is written below as Eq. 3.1, and its components and units are given in Table 3.2.

$$\begin{aligned} E^P = E^0 - \mu^0_\alpha F_\alpha - \frac{1}{2}\alpha_{\alpha\beta}F_\alpha F_\beta - \frac{1}{6}\beta_{\alpha\beta\gamma}F_\alpha F_\beta F_\gamma - \frac{1}{24}\gamma_{\alpha\beta\gamma\delta}F_\alpha F_\beta F_\gamma F_\delta \\ - \frac{1}{3}\Theta^0_{\alpha\beta}F_{\alpha\beta} - \frac{1}{3}A_{\gamma,\alpha\beta}F_\gamma F_{\alpha\beta} - \frac{1}{6}B_{\alpha\beta,\gamma\delta}F_\alpha F_\beta F_{\gamma\delta} - \frac{1}{6}C_{\alpha\beta,\gamma\delta}F_{\alpha\beta}F_{\gamma\delta} - ... \end{aligned} \tag{3.1}$$

Since carbon dioxide is a symmetric molecule, any terms in Eq. 3.1 with an odd number of indices (and an odd-powered field term) will be zero, while the ones with an even number of indices will not: CO_2 does not have a first hyperpolarizability, which is the cubic response to the electric field, but it does have a second hyperpolarizability, which is the quartic response. Although there are higher order terms, as we will discuss in Section 4.1, they do not contribute to the energy at the electric fields we have used and can therefore be excluded from the equation. F_α is the electric field in a given direction, and $F_{\alpha\beta}$ is the field gradient, which is the derivative of the field in direction α with respect to direction β. Using a dipolar electric field makes $F_{\alpha\beta}$ zero, thus Eq. 3.1 can be simplified to Eq. 3.2.

$$E^P = E^0 - \frac{1}{2}\alpha_{\alpha\beta}F_\alpha F_\beta - \frac{1}{24}\gamma_{\alpha\beta\gamma\delta}F_\alpha F_\beta F_\gamma F_\delta \tag{3.2}$$

This equation is written in Einstein summation notation, where repeated Greek subscripts represent a summation of the directional components of the field (x and z in this work). Expanding each term accordingly, canceling out any non-symmetric terms as we did previously, and summing any like terms reduces Eq. 3.2 to Eq. 3.3.

$$E^P - E^0 = -\frac{1}{2}[\alpha_{xx}F_x^2 + \alpha_{zz}F_z^2] - \frac{1}{24}[\gamma_{xxxx}F_x^4 + 6\gamma_{xxzz}F_x^2F_z^2 + \gamma_{zzzz}F_z^4] \tag{3.3}$$

3.2.3 Solving for the Polarizabilities and Hyperpolarizabilities

Using Eq. 3.3, the polarizability and hyperpolarizability can be calculated by placing a carbon dioxide molecule in an electric field in the x-, xz-, and z-directions as shown in Figure 3.1. When the molecule is in the xz-direction, it is placed at a 45° angle so that the F_x and

Table 3.2: The components of Eq. 3.1.

Symbol	Description	Atomic Units
E^P	Energy in an electric field	E_H
E^0	Energy in no electric field	E_H
F_α	Field in the direction α	$\frac{E_H}{ea_0}$
μ^0_α	Permanent dipole moment	ea_0
Θ^0	Permanent quadrupole moment	ea_0^2
α	Polarizability	$\frac{e^2a_0^2}{E_H}$
β	First hyperpolarizability	$\frac{e^3a_0^3}{E_H^3}$
γ	Second hyperpolarizability	$\frac{e^4a_0^4}{E_H^3}$
A, B, C	Field gradient polarizabilities	Varies
$F_{\alpha\beta}$	Field gradient	$\frac{E_H}{ea_0^2}$

F_z values are equivalent. When the molecule is in the x-direction, any F_z terms become zero, leaving only the α_{xx} and γ_{xxxx} values (Eq. 3.4); correspondingly, when the molecule is in the z-direction, the α_{zz} and γ_{zzzz} terms are left (Eq. 3.5).

$$E^P - E^0 = -\frac{1}{2}\alpha_{xx}F_x^2 - \frac{1}{24}\gamma_{xxxx}F_x^4 \tag{3.4}$$

$$E^P - E^0 = -\frac{1}{2}\alpha_{zz}F_z^2 - \frac{1}{24}\gamma_{zzzz}F_z^4 \tag{3.5}$$

When the difference in the energy of the molecule in an electric field and in no electric field is plotted versus the field strength, the fitting function is of the form Eq. 3.6. The coefficient of the x^2 term is the α_{xx} value, and the coefficient of the x^4 term is the γ_{xxxx} value when the molecule is in the x-direction; similar calculations can be done when the molecule is in the z-direction. The γ_{xxzz} term is more difficult to solve for as there is an F_x and F_z component; however, the same method can be used to obtain the coefficient of the x^4 term, which corresponds to the hyperpolarizability portion of Eq. 3.3. The values obtained from the x-direction and the z-direction can then be used to calculate γ_{xxzz}.

$$\Delta E = ax^2 + bx^4 \tag{3.6}$$

The polarizabilities and hyperpolarizabilities can also be calculated from the induced dipole moment of a carbon dioxide monomer. Taking the negative derivative of Eq. 3.3 with respect to the x-direction produces Eq. 3.7, while doing the same with respect to the z-direction produces Eq. 3.8. As before, the molecule is placed in an electric field, and the dipole moment is then used to solve for the polarizabilities and hyperpolarizabilities through the use of fitting equations. The polarizabilities can then be used to solve for a function describing the interaction-induced dipole moments of $(CO_2)_2$.

$$\mu^P = \frac{1}{2}(2\alpha_{xx}F_x) + \frac{1}{24}(4\gamma_{xxxx}F_x^3 + 12F_z^2\gamma_{xxzz}F_x) \tag{3.7}$$

$$\mu^P = \frac{1}{2}(2\alpha_{zz}F_z) + \frac{1}{24}(4\gamma_{zzzz}F_z^3 + 12F_x^2\gamma_{xxzz}F_z) \tag{3.8}$$

3.3 Calculating the Interaction-Induced Dipole Moment of $(CO_2)_2$

The interaction-induced dipole moments of $(CO_2)_2$ can be calculated using Eq. 3.9 [23], which consists of the induction operator $A_{\lambda_1\lambda_2\Lambda L}(r, r_1, r_2)$ (Eq. 3.14) and the spherical harmonics component $Y^{1\nu}_{\lambda_1\lambda_2\Lambda L}(\Omega_1, \Omega_2, \Omega)$ (Eq. 3.10). The $\lambda_1\lambda_2\Lambda L$ term is a set of rotational states: the possible values for the CO_2 dimer are 2023, 0223, 2233, 4045, and 0445 [5]. The dipole moment μ_ν is the dipole moment in the direction ν. The z-direction corresponds to $\nu = 0$, and the x- and y-directions correspond to $\nu = \pm 1$.

$$\mu_\nu(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = \frac{(4\pi)^{\frac{3}{2}}}{\sqrt{3}} \sum_{\lambda_1\lambda_2\Lambda L} A_{\lambda_1\lambda_2\Lambda L}(r, r_1, r_2) Y^{1\nu}_{\lambda_1\lambda_2\Lambda L}(\Omega_1, \Omega_2, \Omega) \tag{3.9}$$

3.3.1 Solving the Spherical Harmonics Portion

The spherical harmonics portion of Eq. 3.9 is described by Eq. 3.10 [5]. $C(\lambda_1\lambda_2\Lambda; M_1M_2M_\Lambda)$ and $C(\Lambda L1; M_\Lambda M\nu)$ are Clebsch-Gordan coefficients; $Y_{\lambda_1 M_1}(\Omega_1)$, $Y_{\lambda_2 M_2}(\Omega_2)$, and $Y_{LM}(\Omega)$ are the spherical harmonics of the first molecule in the dimer, the second molecule in the dimer, and the joining vector between them; and M, M_1, M_2, and M_Λ are values that are related to L, λ_1, λ_2, and Λ, respectively, by the relationships listed in Eq. 3.11.

Each Ω value consists of two angles, θ and ϕ. This equation can be used for any dimer geometry, but for this work, the only dimer configuration studied was the T-shaped dimer. In this particular dimer geometry, where the second molecule is at a 90° angle to the first, the θ and ϕ angles for Molecule 1, Molecule 2, and the joining vector are as follows: $\theta_1 = 0°$, $\phi_1 = 0°$; $\theta_2 = 90°$, $\phi_2 = 0°$; $\theta = 0°$, $\phi = 0°$.

$$\begin{aligned} Y^{1\nu}_{\lambda_1\lambda_2\Lambda L}(\Omega_1, \Omega_2, \Omega) = \sum_{MM_1M_2M_\Lambda} & C(\lambda_1\lambda_2\Lambda; M_1M_2M_\Lambda) C(\Lambda L1; M_\Lambda M\nu) \\ & \times Y_{\lambda_1 M_1}(\Omega_1) Y_{\lambda_2 M_2}(\Omega_2) Y_{LM}(\Omega) \end{aligned} \tag{3.10}$$

$$M_1 = -\gamma_1, \ldots, +\gamma_1 \tag{3.11a}$$

$$M_2 = -\gamma_2, \ldots, +\gamma_2 \tag{3.11b}$$

$$M = -L, \ldots, +L \tag{3.11c}$$

$$M_\Lambda = -\Lambda, \ldots, +\Lambda \tag{3.11d}$$

$$M_1 + M_2 = M_\Lambda \tag{3.11e}$$

$$M_\Lambda + M = \nu \tag{3.11f}$$

Equation 3.10 was solved for each set of induction operators when $\nu = 0$, +1, and -1. For $\nu = +1$ and -1, all of the spherical harmonics were zero. At $\nu = 0$, the 2233 induction operator was zero, leaving only the 2023, 0223, 4045, and 0445 coefficients. These values were then used in Eq. 3.9 to form Eq. 3.12. Since $A_{2023} = -A_{0223}$ and $A_{4045} = -A_{0445}$, this equation could then be simplified to Eq. 3.13.

$$\mu_\nu(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = \frac{(4\pi)^{\frac{3}{2}}}{\sqrt{3}}\left(\frac{3}{8\pi\sqrt{\pi}}A_{2023} + \frac{3}{16\pi\sqrt{\pi}}A_{0223} + \frac{\sqrt{15}}{8\pi\sqrt{\pi}}A_{4045} + \frac{3\sqrt{15}}{64\pi\sqrt{\pi}}A_{0445}\right) \tag{3.12}$$

$$\mu_\nu(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = \frac{3\sqrt{3}}{2}A_{2023} + \frac{5\sqrt{5}}{8}A_{4045} \tag{3.13}$$

3.3.2 Solving the Induction Operator Portion

After simplifying the spherical harmonics portion, the induction operator portion can be expanded. The induction operator is given by Eq. 3.14, where $B^{(m)}_{\lambda_1\lambda_2\Lambda L}$ is a value that changes depending on $\lambda_1\lambda_2\Lambda L$ and is composed of the polarizability and the quadrupole moment for the 2023 term or the polarizability and the hexadecapole moment for the 4045 term. The value of m in r^m is also dependent upon $\lambda_1\lambda_2\Lambda L$. The distance between the carbons in the dimer is r. $\mu_{\lambda_1\lambda_2\Lambda L}$ and $\mathrm{r}_{\lambda_1\lambda_2\Lambda L}$ are constants, and σ is the value of r when

the potential is zero. Substituting this equation into Eq. 3.13 and using the m values from El-Kader and Maroulis [5] creates Eq. 3.15. Using the constants from El-Kader and Maroulis [5], Eq. 3.16 gives an expression for the interaction-induced dipole moments.

$$A_{\lambda_1\lambda_2\Lambda L}(r) = \frac{B^{(m)}_{\lambda_1\lambda_2\Lambda L}}{r^m} + \mu_{\lambda_1\lambda_2\Lambda L}\exp(-\frac{r-\sigma}{r_{\lambda_1\lambda_2\Lambda L}}) \tag{3.14}$$

$$\begin{aligned}\mu_\nu(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = \frac{3\sqrt{3}}{2}\left[\frac{B_{2023}}{r^4} + \mu_{2023}\exp(-\frac{r-\sigma}{r_{2023}})\right] \\ + \frac{5\sqrt{5}}{8}\left[\frac{B_{4045}}{r^6} + \mu_{4045}\exp(-\frac{r-\sigma}{r_{4045}})\right]\end{aligned} \tag{3.15}$$

$$\begin{aligned}\mu_0(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = -\frac{281.138}{r^4} - \frac{129.468}{r^6} \\ - 0.304\exp(-\frac{r-7.0562}{1.342}) - 0.0264\exp(-\frac{r-7.0562}{0.561})\end{aligned} \tag{3.16}$$

3.3.3 *ab initio* Dipole Calculations

The values used in Eq. 3.16 were based on experimental and semi-empirical results. However, the goal of this work is to use only *ab initio* results. At the RHF and MP2 levels of theory, the dipole moment is given directly. At the CCSD and CCSD(T) levels of theory, however, the finite-field method must be used. The energy of the dimer at a particular value of r is calculated at multiple field strengths; then the energies are plotted against the field strengths and fit to either a linear or a quadratic function. The negative first derivative of this function at F=0 is the dipole moment. The dipole moments reported in Chapter 5 were calculated using both a linear and a quadratic fit, which at F=0 gave the same results.

The dipole moments then had to be counterpoise corrected [2] to account for the basis set superposition error (BSSE). When calculating the energy of a dimer, the basis functions of one molecule can contribute to the other molecule, and vice versa. To account for this, we calculated the energy and dipole moment when the first molecule is comprised of ghost atoms, and then again when the second molecule is comprised of ghost atoms [32]. Ghost atoms are formed of only the basis functions of the true atom without including electrons.

The "ghost" dipole moments were then subtracted from the dipole moment of the complete dimer. The corrected dipole moments were plotted versus r, and a modified version of Eq. 3.15 was used to fit the points as described in Section 5.2.2.

Chapter 4

Monomer Results

The first portion of this work calculated the polarizability and hyperpolarizability of carbon dioxide, along with the quadrupole and hexadecapole moments. Calculating accurate properties is important as these values will be used to calculate the interaction-induced dipole moments of a carbon dioxide dimer. Ensuring that the results for a monomer are accurate will help us achieve accurate results for the dimer. To begin, we first found what field strengths, basis sets, and bond lengths were needed to get accurate results. Then we performed high-level *ab initio* calculations to determine α_{xx}, α_{zz}, γ_{xxxx}, γ_{xxzz}, and γ_{zzzz}, and compared these results to literature. Unless specified otherwise, all results were obtained using the GAMESS *ab initio* software package [29, 8, 26].

4.1 Effect of Field Strength on CO_2

The calculations of the response properties rely on the difference in energy between an unperturbed carbon dioxide molecule and a carbon dioxide molecule perturbed by an electric field; therefore, it is important to determine which field strengths are appropriate to use. In Eq. 3.3, the equation was truncated at the quartic term, which corresponds to the second hyperpolarizability, and higher order terms are disregarded. As the field strength increases, we expect to see contributions from terms higher than the fourth order. Consequently, it is important to only consider field strengths where there are minimal contributions from higher-order terms.

4.1.1 Initial Field Strength Investigation

To get an idea of how large the field strength would need to be, a carbon dioxide molecule was placed in an electric field in the x-, xz-, and z-directions. The field was increased from 0.0 au, and the energy was calculated. To find the equilibrium bond length of CO_2, the rotational constant from Ref. [35] was used [19]. The bond length was found to be 1.15995 Å, and all calculations were performed at this bond length unless otherwise noted. For the field strength calculations, the RHF and MP2 levels of theory were used with the ACCT basis set.

Selected results of this investigation are listed in Table 4.1, and the complete results are in Appendix A.1. At a field strength of 0.110 au for the molecule in the z-direction, the energy was unable to converge at the RHF level of theory. Therefore, all further calculations will be kept below 0.11 au.

4.1.2 Calculating γ_{xxzz} from Exact Properties

After finding the maximum possible field strength for the CO_2 molecule, the field strength at which there was no significant contribution from terms higher than the fourth order could be determined. At the RHF level of theory, the polarizabilities and hyperpolarizabilities can be directly calculated. Using these polarizability and hyperpolarizability values, γ_{xxzz} can be calculated using Eq. 3.3 and compared to the exact values.

A carbon dioxide molecule at the equilibrium bond length was placed in an electric field in the xz-direction, and the energy, polarizabilities, and hyperpolarizabilities were calculated using RHF with the ACCD, ACCT, and ACCQ basis sets. The α_{xx}, α_{zz}, γ_{xxxx}, and γ_{zzzz} values in no electric field were used in Eq. 3.3. Field strengths up to 0.06 au were tested, and the difference between the unperturbed molecule and the perturbed molecule at these various fields were used to calculate γ_{xxzz}. The exact polarizabilities and hyperpolarizabilities from the RHF calculations are listed in Table 4.2, and the calculated ACCQ γ_{xxzz} values are in Table 4.3. The ACCD and ACCT results are listed in Tables A.2 and A.3 in Appendix A.2.

$$E^P - E^0 = -\frac{1}{2}[\alpha_{xx}F_x^2 + \alpha_{zz}F_z^2] - \frac{1}{24}[\gamma_{xxxx}F_x^4 + 6\gamma_{xxzz}F_x^2F_z^2 + \gamma_{zzzz}F_z^4] \tag{3.3}$$

Table 4.1: MP2 energies of a carbon dioxide molecule in selected fields in the x-, xz-, and z-directions.

Fields	X	XZ	Z
0.000	−188.321 230	−188.321 230	−188.321 230
0.005	−188.321 372	−188.321 472	−188.321 572
0.010	−188.321 797	−188.322 198	−188.322 599
0.050	−188.335 537	−188.345 602	−188.355 725
0.100	−188.380 564	−188.422 428	−188.465 261

Table 4.2: The exact RHF polarizabilities, hyperpolarizabilities, and energy for a CO_2 molecule in the xz-direction.

Property	ACCD	ACCT	ACCQ
Energy	−187.662 832	−187.709 518	−187.722 229
α_{xx}	11.2640	11.8073	11.9387
α_{zz}	23.6459	23.6553	23.6508
γ_{xxxx}	413.9433	534.4799	634.5364
γ_{xxzz}	213.4673	259.7815	307.3156
γ_{zzzz}	547.8861	697.6962	792.3639

Table 4.3: The calculated energies and the γ_{xxzz} values and errors for a carbon dioxide molecule in the xz-direction for the ACCQ basis set.

Field Strength	Energy	γ_{xxzz}	Percent Error
0.0025	−187.722 284	306.1849	0.368
0.0050	−187.722 451	307.7837	0.152
0.0075	−187.722 729	308.5853	0.413
0.0100	−187.723 119	309.3033	0.647
0.0125	−187.723 620	310.3940	1.002
0.0150	−187.724 233	311.7023	1.427
0.0175	−187.724 957	313.2886	1.944
0.0200	−187.725 793	315.1633	2.554
0.0225	−187.726 742	317.3301	3.259
0.0250	−187.727 803	319.7968	4.061
0.0275	−187.728 978	322.5892	4.970
0.0300	−187.730 265	325.7220	5.989
0.0350	−187.733 182	333.1295	8.400
0.0400	−187.736 557	342.2902	11.381
0.0450	−187.740 398	353.6030	15.062
0.0500	−187.744 709	367.6554	19.634
0.0550	−187.749 500	385.3684	25.398
0.0600	−187.754 783	408.2602	32.847

The percent error of the calculated γ_{xxzz} increased as the field strength increased. The largest percent error occurred at the largest field strength for each basis set, which is most likely due to contributions to the energy from higher order terms. Similarly, at the lowest field strength of 0.0025 au, the percent error was larger than the next highest field of 0.005 au due to the field being too small to capture the quartic term. All further calculations were performed at field strengths between 0.005 au and 0.02 au.

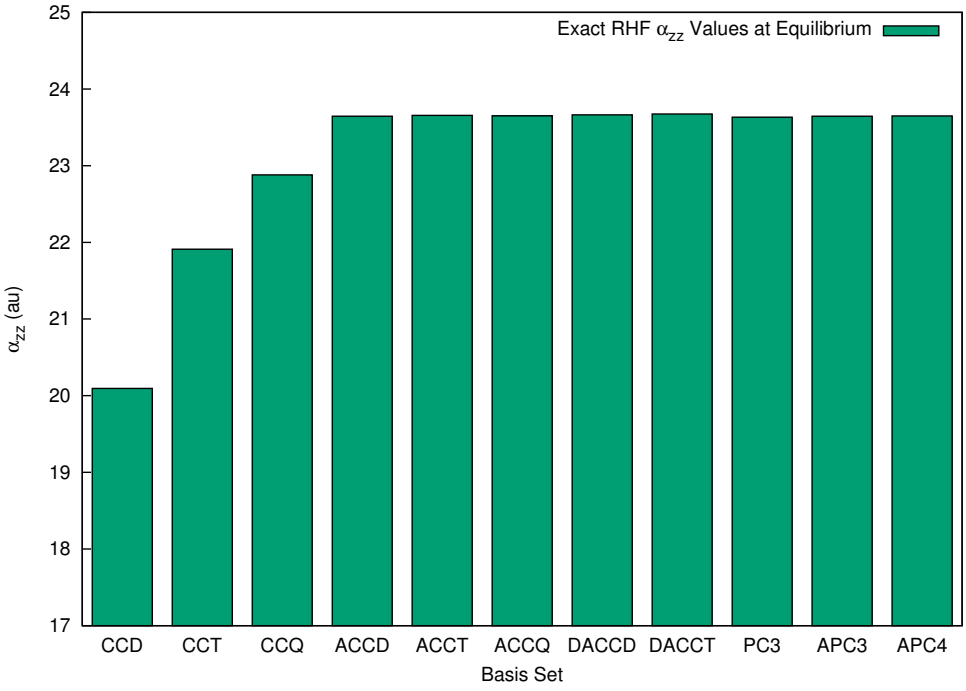
4.2 Effect of Basis Set and Bond Length

4.2.1 Basis Set Analysis

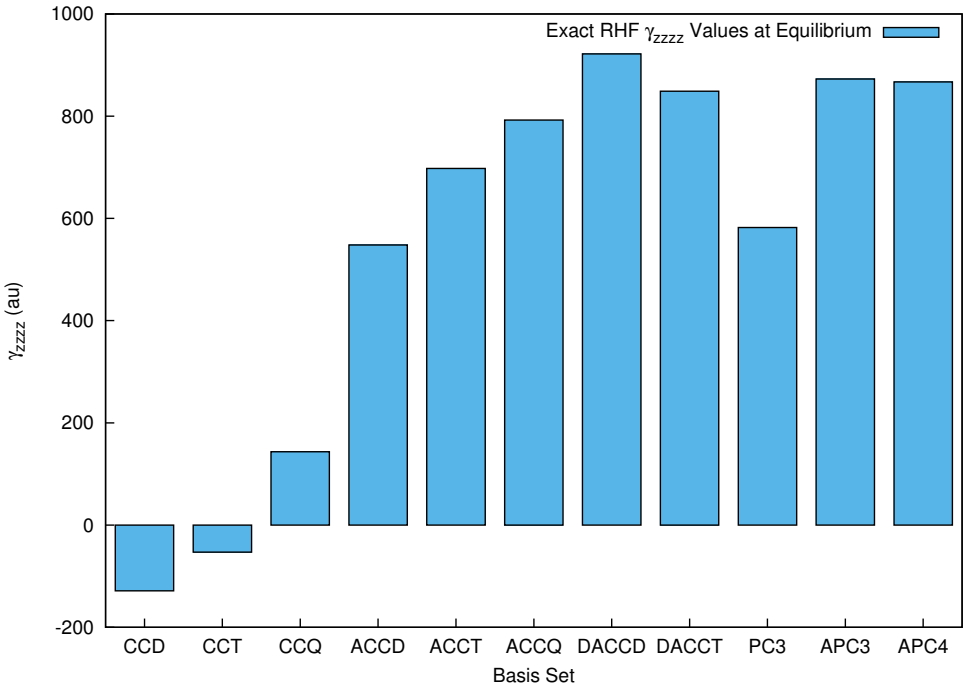
After finding which field strengths can be used, we next determined which basis sets to use. We began by testing the eleven basis sets listed in Table 3.1. For each basis set, the energy, dipole moment, polarizabilities, and hyperpolarizabilities were calculated using RHF and compared to one another. In Figure 4.1a, the α_{zz} values obtained directly from the RHF calculations are shown. As the basis sets get larger, the value of α_{zz} converges to approximately 23.65 au. The addition of the diffuse functions are important as seen in the dramatic increase from the CCD to the ACCD basis set. Adding an additional diffuse function does not affect the value significantly. The PC3 basis set result is on par with the augmented basis sets, showing that it does give comparable results to the larger and more expensive basis sets.

However, this same behavior is not seen in the hyperpolarizability values. The non-augmented basis sets perform significantly worse when calculating the γ_{zzzz} value, with the notable exception of PC3 performing on par with the ACCD basis set. There is a difference in the value when using the doubly augmented basis sets, DACCD and DACCT, but as seen in Figure 4.1b, there is no clear convergence in the γ_{zzzz} values as there was in the α_{zz} values.

As a result, we will use the ACCT, ACCQ, and APC3 basis sets for the MP2, CCSD, and CCSD(T) calculations. The ACCT basis is relatively small, so calculations at higher levels of theory should complete quickly. The ACCQ basis set is larger than the ACCT basis set, so it should give more accurate results as there are more functions describing the



(a) α_{zz} Values



(b) γ_{zzzz} Values

Figure 4.1: The α_{zz} and γ_{zzzz} values of a carbon dioxide monomer at the equilibrium bond length of 1.15995 Å. The values were obtained from RHF calculations using the basis sets listed.

orbitals of each atom. The APC3 basis set gave hyperpolarizability results on par with the APC4 basis set, but as it is smaller than the APC4 basis set, its calculations will not be as computationally intensive.

4.2.2 Bond Length Analysis

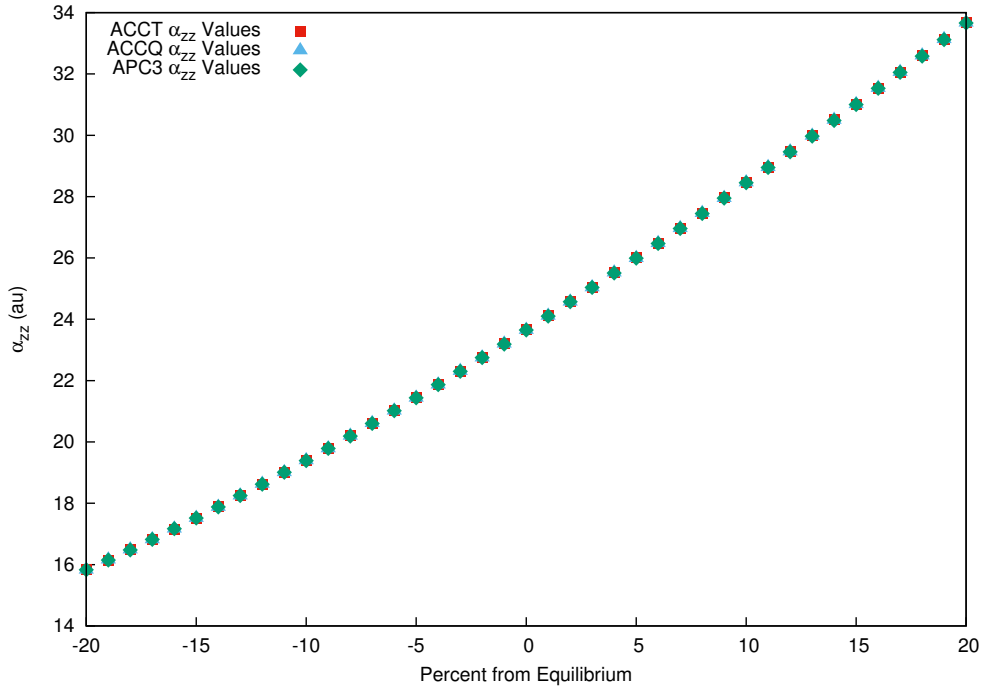
In addition to determining which basis sets were suitable to use, we also investigated the effect of changing the bond length on the response properties. For each of the basis sets, a carbon dioxide molecule was displaced from equilibrium by ± 20% in increments of 1%, and the energies, polarizabilities, and hyperpolarizabilities were directly calculated. No electric field was used for these calculations. Some of the results for the ACCT, ACCQ, and APC3 basis sets are in Table 4.4, and the full set of results is in Appendix A.3. In Figure 4.2a, the α_{zz} values for three basis sets (ACCT, ACCQ, and APC3) are nearly indistinguishable, and the values are close to linear. Conversely, in Figure 4.2b, the γ_{zzzz} values for the three basis sets are distinct. The smallest basis set, ACCT, returned the lowest γ_{zzzz} values, whereas the largest basis set, APC3, returned the highest values. As the bond is stretched, the values deviate from a linear fit and increase at a faster rate. Similar results were seen for the α_{xx}, γ_{xxxx}, and γ_{xxzz} values.

At the RHF level of theory, the calculations are computationally inexpensive. Moving to higher levels of theory requires more computational time and resources, which makes using all forty-one bond lengths for higher-level calculations unfeasible. For that reason, a subset of bond lengths which still captures the behavior of all points must be determined. To accomplish this, we divided the bond lengths into five sets: ±0,5,10,15,20%; ±0,4,8,12,16,20%; ±0,6,12,18%; ±0,7,14,20%; and ±0,3,9,15,20%. Next, the response properties versus the bond lengths were fit to the five polynomials in Eq. 4.1, and the maximum error and the percent error relative to the exact response property were calculated.

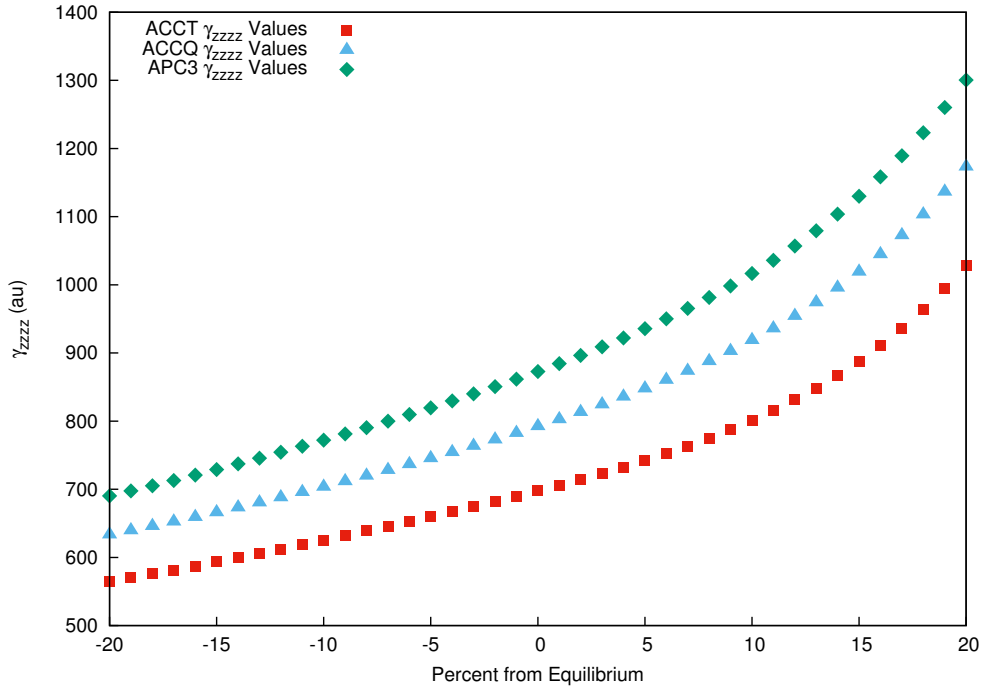
The subset that was found to have errors on par with the complete set whilst minimizing the amount of points needed was the ±0,6,12,18% set. The fitting results of the α_{zz} and γ_{zzzz} values calculated with the ACCT, ACCQ, and APC3 basis sets for this subset are listed in Tables 4.5 and 4.6, and the complete set of fitting results is listed in Appendix B.

Table 4.4: Properties of a CO_2 molecule at various bond lengths and basis sets at the RHF level of theory.

Basis Set	Bond Length	Percent	Energy	α_{xx}	α_{zz}	γ_{xxxx}	γ_{xxzz}	γ_{zzzz}
	0.951 16	−18.0	−187.450 754	9.3408	16.4809	310.5999	179.1207	575.7183
	1.020 76	−12.0	−187.626 233	10.1475	18.6226	373.0889	198.7402	612.3091
	1.090 35	−6.00	−187.700 619	10.9740	21.0229	448.3105	225.4333	652.7964
ACCT	1.159 95	0.00	−187.709 518	11.8073	23.6553	534.4799	259.7815	697.6962
	1.229 55	6.00	−187.677 335	12.6343	26.4840	629.6211	302.8961	752.3323
	1.299 14	12.0	−187.620 957	13.4412	29.4704	731.3642	356.9431	831.0936
	1.368 74	18.0	−187.552 161	14.2124	32.5921	836.8733	425.7502	963.8516
	0.951 16	−18.0	−187.468 648	9.4239	16.4856	374.9376	214.9497	645.8469
	1.020 76	−12.0	−187.641 886	10.2451	18.6257	447.1752	238.1638	687.9924
	1.090 35	−6.00	−187.714 550	11.0880	21.0222	534.2999	268.6876	736.5965
ACCQ	1.159 95	0.00	−187.722 229	11.9387	23.6508	634.5364	307.3156	792.3639
	1.229 55	6.00	−187.689 220	12.7837	26.4784	745.5023	355.3269	860.3556
	1.299 14	12.0	−187.632 293	13.6086	29.4676	864.2655	414.8955	954.2649
	1.368 74	18.0	−187.563 123	14.3984	32.5964	987.4938	489.8975	1103.1056
	0.951 16	−18.0	−187.471 065	9.4340	16.4850	442.7228	246.5232	705.0808
	1.020 76	−12.0	−187.644 024	10.2558	18.6236	529.9112	275.1676	754.2611
	1.090 35	−6.00	−187.716 483	11.1003	21.0184	635.6840	312.3034	809.6163
APC3	1.159 95	0.00	−187.723 987	11.9536	23.6451	758.0617	358.4271	872.7582
	1.229 55	6.00	−187.690 835	12.8018	26.4703	894.5732	414.6826	950.1375
	1.299 14	12.0	−187.633 798	13.6308	29.4572	1042.2151	483.2359	1056.9074
	1.368 74	18.0	−187.564 541	14.4253	32.5846	1197.4121	568.0545	1223.2609



(a) α_{zz} Values



(b) γ_{zzzz} Values

Figure 4.2: The α_{zz} and γ_{zzzz} values calculated at the RHF level using the ACCT, ACCQ, and APC3 basis sets.

Table 4.5: The fitting coefficients and errors for the ACCT, ACCQ, and APC3 basis sets for the α_{zz} values.

	ACCT		ACCQ		APC3	
Coefficients	0,6,12,18	All Points	0,6,12,18	All Points	0,6,12,18	All Points
a	23.66		23.65		23.65	
b_1	0.449	0.449	0.449	0.449	0.449	0.449
b_2	0.449	0.449	0.449	0.449	0.449	0.449
b_3	0.456	0.456	0.455	0.455	0.455	0.455
b_4	0.456	0.456	0.455	0.455	0.455	0.455
b_5	0.456	0.456	0.456	0.456	0.455	0.455
c_2	2.72×10^{-3}	2.72×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_3	2.72×10^{-3}	2.72×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_4	2.72×10^{-3}	2.71×10^{-3}	2.75×10^{-3}	2.74×10^{-3}	2.75×10^{-3}	2.74×10^{-3}
c_5	2.72×10^{-3}	2.71×10^{-3}	2.75×10^{-3}	2.74×10^{-3}	2.75×10^{-3}	2.74×10^{-3}
d_3	-2.54×10^{-5}	-2.48×10^{-5}	-2.41×10^{-5}	-2.34×10^{-5}	-2.39×10^{-5}	-2.32×10^{-5}
d_4	-2.54×10^{-5}	-2.48×10^{-5}	-2.41×10^{-5}	-2.34×10^{-5}	-2.39×10^{-5}	-2.32×10^{-5}
d_5	-3.11×10^{-5}	-3.14×10^{-5}	-2.96×10^{-5}	-2.99×10^{-5}	-2.94×10^{-5}	-2.97×10^{-5}
e_4	9.51×10^{-9}	4.03×10^{-8}	-1.43×10^{-8}	1.78×10^{-8}	-1.21×10^{-10}	3.06×10^{-8}
e_5	9.51×10^{-9}	4.03×10^{-8}	-1.43×10^{-8}	1.78×10^{-8}	-1.21×10^{-10}	3.06×10^{-8}
g_5	1.36×10^{-8}	1.43×10^{-8}	1.31×10^{-8}	1.39×10^{-8}	1.31×10^{-8}	1.38×10^{-8}
$RMSE_1$	0.512	0.512	0.517	0.517	0.517	0.517
$RMSE_2$	0.032	0.032	0.030	0.030	0.030	0.030
$RMSE_3$	2.38×10^{-3}	2.16×10^{-3}	2.24×10^{-3}	2.03×10^{-3}	2.27×10^{-3}	2.05×10^{-3}
$RMSE_4$	2.34×10^{-3}	2.05×10^{-3}	2.29×10^{-3}	2.00×10^{-3}	2.27×10^{-3}	1.99×10^{-3}
$RMSE_5$	8.71×10^{-4}	6.29×10^{-4}	9.10×10^{-4}	6.59×10^{-4}	8.71×10^{-4}	6.28×10^{-4}
Percent Error 1	7.326	7.330	7.366	7.370	7.360	7.364
Percent Error 2	0.453	0.453	0.423	0.424	0.423	0.423
Percent Error 3	0.032	0.023	0.029	0.020	0.030	0.021
Percent Error 4	0.031	0.018	0.031	0.018	0.030	0.017
Percent Error 5	0.011	4.45×10^{-3}	0.012	4.65×10^{-3}	0.012	4.47×10^{-3}

Table 4.6: The fitting coefficients and errors for the ACCT, ACCQ, and APC3 basis sets for the γ_{zzzz} values.

	ACCT		ACCQ		APC3	
Coefficients	0,6,12,18	All Points	0,6,12,18	All Points	0,6,12,18	All Points
a	697.70		792.36		872.76	
b_1	10.128	10.138	12.072	12.082	13.693	13.702
b_2	10.128	10.138	12.072	12.082	13.693	13.702
b_3	7.866	7.812	9.893	9.839	11.262	11.210
b_4	7.866	7.812	9.893	9.839	11.262	11.210
b_5	8.051	8.050	10.083	10.082	11.438	11.439
c_2	0.212	0.215	0.244	0.246	0.272	0.275
c_3	0.212	0.215	0.244	0.246	0.272	0.275
c_4	0.122	0.121	0.157	0.156	0.185	0.183
c_5	0.122	0.121	0.157	0.156	0.185	0.183
d_3	8.98×10^{-3}	9.23×10^{-3}	8.65×10^{-3}	8.91×10^{-3}	9.65×10^{-3}	9.90×10^{-3}
d_4	8.98×10^{-3}	9.23×10^{-3}	8.65×10^{-3}	8.91×10^{-3}	9.65×10^{-3}	9.90×10^{-3}
d_5	6.58×10^{-3}	6.58×10^{-3}	6.18×10^{-3}	6.19×10^{-3}	7.35×10^{-3}	7.34×10^{-3}
e_4	3.09×10^{-4}	3.14×10^{-4}	2.97×10^{-4}	3.03×10^{-4}	3.00×10^{-4}	3.06×10^{-4}
e_5	3.09×10^{-4}	3.14×10^{-4}	2.97×10^{-4}	3.03×10^{-4}	3.00×10^{-4}	3.06×10^{-4}
g_5	5.72×10^{-6}	5.70×10^{-6}	5.87×10^{-6}	5.84×10^{-6}	5.47×10^{-6}	5.51×10^{-6}
$RMSE_1$	42.471	42.471	47.963	47.962	53.467	53.467
$RMSE_2$	13.108	13.098	12.645	12.635	13.843	13.833
$RMSE_3$	5.337	5.301	5.154	5.117	5.194	5.159
$RMSE_4$	0.869	0.785	0.890	0.804	0.844	0.761
$RMSE_5$	0.147	0.107	0.162	0.118	0.167	0.121
Percent Error 1	12.472	12.453	11.884	11.867	11.829	11.815
Percent Error 2	4.208	4.085	3.571	3.465	3.450	3.354
Percent Error 3	1.624	1.424	1.390	1.215	1.254	1.099
Percent Error 4	0.323	0.196	0.293	0.177	0.255	0.154
Percent Error 5	0.101	0.043	0.101	0.042	0.050	0.021

$$y_1 = b_1 x + a \tag{4.1a}$$

$$y_2 = c_2 x^2 + b_2 x + a \tag{4.1b}$$

$$y_3 = d_3 x^3 + c_3 x^2 + b_3 x + a \tag{4.1c}$$

$$y_4 = e_4 x^4 + d_4 x^3 + c_4 x^2 + b_4 x + a \tag{4.1d}$$

$$y_5 = f_5 x^5 + e_5 x^4 + d_5 x^3 + c_5 x^2 + b_5 x + a \tag{4.1e}$$

4.3 Calculating the Response Properties at Higher Levels of Theory

Now that the choice of field strengths, basis sets, and bond lengths have been determined, we can use higher levels of theory to calculate the polarizabilities and hyperpolarizabilities. At the MP2, CCSD, and CCSD(T) levels of theory, the polarizabilities and hyperpolarizabilities can not be directly calculated. Instead, the method discussed in Section 3.2.3 was used to solve for α_{xx}, α_{zz}, γ_{xxxx}, γ_{xxzz}, and γ_{zzzz}. A carbon dioxide molecule was placed in an electric field in the x, xz, and z-directions, and Eqs. 3.3, 3.4, and 3.5 were used to calculate the polarizabilities and hyperpolarizabilities. At the RHF and MP2 levels of theory, the dipole moment can be calculated and used in Eqs. 3.7 and 3.8 to solve for the necessary properties, an example of which is shown in Figure 4.3 for the z-direction APC3 RHF dipole moments at the equilibrium bond length.

$$E^P - E^0 = -\frac{1}{2}[\alpha_{xx} F_x^2 + \alpha_{zz} F_z^2] - \frac{1}{24}[\gamma_{xxxx} F_x^4 + 6\gamma_{xxzz} F_x^2 F_z^2 + \gamma_{zzzz} F_z^4] \tag{3.3}$$

$$E^P - E^0 = -\frac{1}{2}\alpha_{xx} F_x^2 - \frac{1}{24}\gamma_{xxxx} \tag{3.4}$$

$$E^P - E^0 = -\frac{1}{2}\alpha_{zz} F_z^2 - \frac{1}{24}\gamma_{xxxx} F_x^4 \tag{3.5}$$

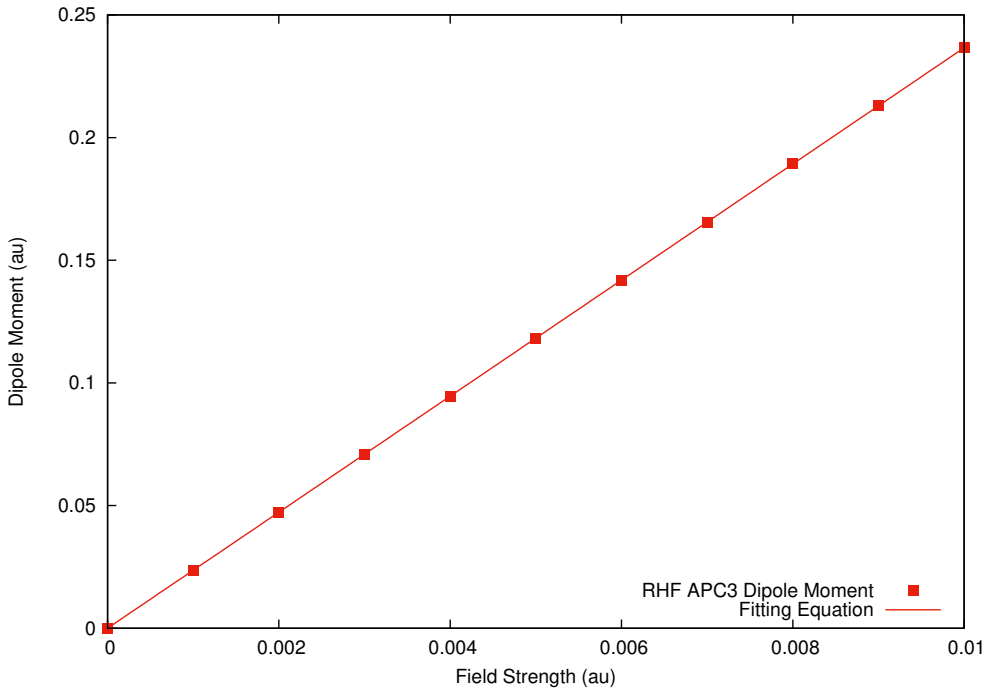


Figure 4.3: The RHF z-direction dipole moments used to calculate the polarizabilities and hyperpolarizabilities for a CO_2 molecule at a bond length of 1.15995 Å using the APC3 basis set.

$$\mu^P = \frac{1}{2}(2\alpha_{xx}F_x) + \frac{1}{24}(4\gamma_{xxxx}F_x^3 + 12F_z^2\gamma_{xxzz}F_x) \tag{3.7}$$

$$\mu^P = \frac{1}{2}(2\alpha_{zz}F_z) + \frac{1}{24}(4\gamma_{zzzz}F_z^3 + 12F_x^2\gamma_{xxzz}F_z) \tag{3.8}$$

From Section 4.1.2, we determined that the field strength used should be between 0.005 and 0.02 au. The electric field was increased from 0.0 to 0.010 au in increments of 0.001 au, and the energies and dipole moments were calculated. The energies at 0.015 and 0.020 au were also calculated and used to solve for α_{xx}, α_{zz}, γ_{xxxx}, γ_{xxzz}, and γ_{zzzz}. Each of the seven bond lengths from Section 4.2.2 were used for every field strength with the ACCT, ACCQ, and APC3 basis sets; the results shown in the below sections are for the equilibrium bond length, and the complete set of energies and dipole moments along with the root mean squared errors of the fits are listed in Appendix A.4, A.5, and A.6.

4.3.1 RHF Calculations and Percent Errors

For the RHF level of theory, the values calculated from the energy can be compared to the exact values obtained directly from the calculations. The percent errors of the calculated values are in Table 4.7. The smallest field strength, 0.005 au, is not included in the results as some of the γ_{xxzz} terms calculated were negative, which is incorrect as the polarizabilities and hyperpolarizabilities must be positive. The errors were the smallest for the α_{xx} and α_{zz} values, which was expected. The γ_{xxzz} terms usually had the largest percent errors due to it being dependent upon the accuracy of the other calculated values. The error across the basis sets and field strengths did not change much, with the ACCT basis set and the 0.02 field strength having on average a larger error.

4.3.2 MP2 and Coupled Cluster Results

The polarizabilities and hyperpolarizabilities were then calculated for the MP2, CCSD, and CCSD(T) levels of theory. Figure 4.4 shows the fit of the z-direction APC3 CCSD(T) energies versus the electric field for carbon dioxide at the equilibrium bond length. The results for

Table 4.7: The percent errors for the properties calculated at the RHF level of theory.

Basis Set	Property	X-Dipole (0.01)	Z-Dipole (0.01)	Energy (0.01)	Energy (0.015)	Energy (0.020)
ACCT	α_{xx}	9.316×10^{-5}	N/A	1.270×10^{-4}	1.694×10^{-5}	5.759×10^{-4}
	α_{zz}	N/A	1.860×10^{-4}	4.354×10^{-4}	2.832×10^{-4}	4.354×10^{-4}
	γ_{xxxx}	0.0380	N/A	0.5376	0.1560	1.1154
	γ_{zzzz}	N/A	0.3659	2.7046	1.2278	1.6295
	γ_{xxzz}	0.4444	0.2489	4.0318	0.9829	2.1484
ACCQ	α_{xx}	1.173×10^{-4}	N/A	1.508×10^{-4}	2.513×10^{-5}	7.455×10^{-4}
	α_{zz}	N/A	3.171×10^{-4}	2.199×10^{-4}	1.987×10^{-4}	4.651×10^{-4}
	γ_{xxxx}	0.1750	N/A	0.0867	0.2925	1.4193
	γ_{zzzz}	N/A	1.0238	1.0257	0.9838	1.6067
	γ_{xxzz}	1.4072	0.7991	3.1288	1.2185	1.9348
APC3	α_{xx}	2.510×10^{-4}	N/A	2.510×10^{-5}	2.008×10^{-4}	9.119×10^{-4}
	α_{zz}	N/A	1.311×10^{-4}	1.649×10^{-4}	3.256×10^{-4}	6.724×10^{-4}
	γ_{xxxx}	0.2805	N/A	0.3871	0.8347	1.7106
	γ_{zzzz}	N/A	0.8948	0.5807	1.5660	2.2989
	γ_{xxzz}	1.4296	0.4871	2.2728	1.0338	3.1675

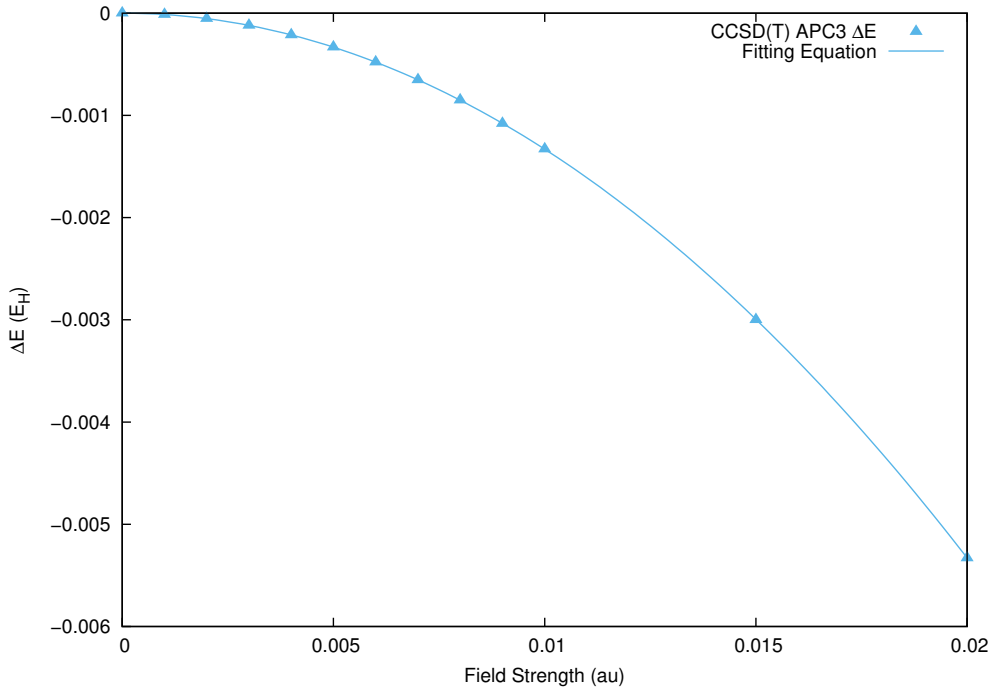


Figure 4.4: The CCSD(T) z-direction energies used to calculate the polarizabilities and hyperpolarizabilities for a CO_2 molecule at a bond length of 1.15995 Å using the APC3 basis set.

the MP2 and CCSD calculations are in Appendix A.7, and the CCSD(T) results are listed below in Table 4.8. The ACCT basis set produced the smallest values, while the APC3 basis set produced the largest, although the polarizabilities were similar for all three basis sets. The hyperpolarizabilities increased by about 100 au between the ACCT and ACCQ basis sets, and similar change was seen between the ACCQ and APC3 hyperpolarizability values. For both the polarizabilities and hyperpolarizabilities, the values across the field strengths were similar, especially between the 0.01 and the 0.015 au results.

4.4 Calculating the Quadrupole and Hexadecapole Moments

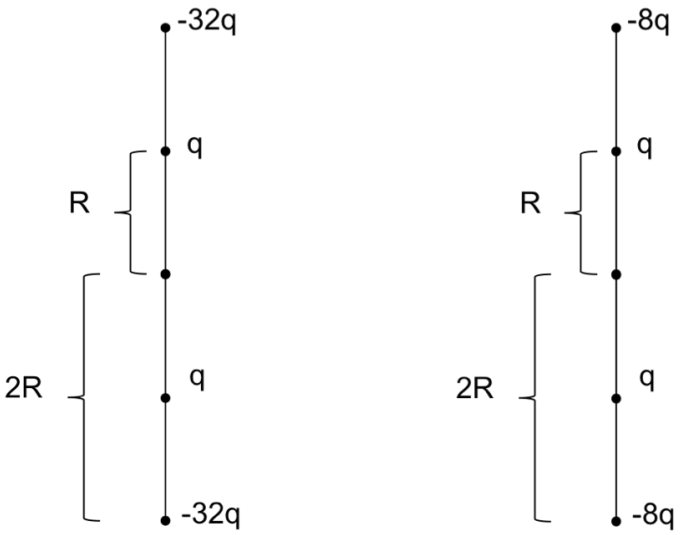
The quadrupole (θ) and hexadecapole (ϕ) moments were also calculated. The NWChem *ab initio* software package was used for this portion of the work [34]. To calculate these values, a carbon dioxide molecule at the equilibrium bond length was placed in the z-direction in an electric field. The field was generated by point charges arranged as shown in Figure 4.5, which is necessary in order to cancel out certain terms in Eq. 3.1 to derive Eqs. 4.2 and 4.3 [21].

The magnitude of one point charge is q, and R is the distance between the origin and the closest point charge. In Eq. 4.2, $E^4(q, R, 0)$ is the energy of the molecule in the electric field as shown in Figure 4.5a, and $E^4(-q, R, 0)$ is the energy when the signs of q are swapped. Similarly, in Eq. 4.3, $E^4(q, R, 0) - E^0$ is the difference in energy between a molecule in the electric field shown in Figure 4.5b and the energy in no electric field. For the quadrupole calculation, $R = 30$ au and $q = 9$ e; for the hexadecapole calculation, $R = 30$ au and $q = 2$ e [21].

The values obtained from these calculations are in Table 4.9. The quadrupole values were similar across the basis sets, but the hexadecapole moments were inconsistent. However, this is expected as the hexadecapole moment is smaller than the quadrupole moment and is thus more difficult to calculate. All units are atomic units.

Table 4.8: Polarizability and hyperpolarizability values of a CO_2 molecule at the equilibrium bond length calculated with the ACCT, ACCQ, and APC3 basis sets at the CCSD(T) level of theory. The maximum field strengths used were 0.01, 0.015, and 0.02 au.

Basis Set	Property	Field = 0.01	Field = 0.015	Field = 0.02
ACCT	α_{xx}	12.6673	12.6673	12.6672
	α_{zz}	26.6950	26.6949	26.6947
	γ_{xxxx}	728.3939	728.5379	735.4433
	γ_{zzzz}	953.3694	985.5131	994.8320
	γ_{xxzz}	374.8139	380.0503	382.5625
ACCQ	α_{xx}	12.7747	12.7747	12.7746
	α_{zz}	26.6171	26.6169	26.6167
	γ_{xxxx}	852.4898	856.9769	861.5357
	γ_{zzzz}	1073.2470	1110.3569	1123.1601
	γ_{xxzz}	447.8922	447.5666	455.2175
APC3	α_{xx}	12.7714	12.7714	12.7713
	α_{zz}	26.6001	26.6002	26.5998
	γ_{xxxx}	1039.3045	1043.9323	1050.6324
	γ_{zzzz}	1255.2692	1252.3962	1277.6850
	γ_{xxzz}	532.3865	537.1431	543.4516



(a) Quadrupole (θ_{zz}) **(b)** Hexadecapole (ϕ_{zzzz})

Figure 4.5: The arrangement of point charges used to calculate θ and ϕ.

Table 4.9: The θ and ϕ values for a carbon dioxide molecule at the equilibrium bond length. RHF, MP2, CCSD, and CCSD(T) calculations were performed with the ACCT, ACCQ, and APC3 basis sets.

	ACCT		ACCQ		APC3	
Theory	θ	ϕ	θ	ϕ	θ	ϕ
RHF	−3.82	−2.05	−3.80	−1.23	−3.80	−1.32
MP2	−3.09	−3.01	−3.07	−2.29	−3.07	−2.45
CCSD	−3.30	−2.79	−3.29	−2.06	−3.29	−2.21
CCSD(T)	−3.19	−3.07	−3.17	−2.36	−3.18	−2.53

$$\theta_{zz} = \frac{R^3 q^{-1}[E^4(-q, R, 0) - E^4(q, R, 0)]}{12} \tag{4.2}$$

$$\phi_{zzzz} = \frac{2}{3} R^5 q^{-1}[E^4(q, R, 0) - E^0] \tag{4.3}$$

4.5 Literature Comparison

4.5.1 Comparison of Theoretical Values

Finally, we compared our values to those previously calculated using methods similar to ones we used. For the polarizability values, we were able to obtain good agreement with values reported by Maroulis [20], Haskopoulos [11], and Kalugina [15] (Table 4.10). Our α_{xx} values agreed within 0.33 au of the literature values; the agreement with the α_{zz} values was within 0.51 au. It is worth noting that the literature values were calculated with different basis sets and bond lengths than what we used, thus differences from the calculated values are expected. Maroulis and Haskopoulos used bespoke basis sets designed for computing these response properties, while Kalugina used a bond length shorter than our equilibrium value with a larger basis set.

The agreement between our hyperpolarizability values was not as great as the polarizability values; the APC3 values agreed best with the DU1 basis set results calculated by Maroulis (Table 4.11). However, the hyperpolarizability values are more sensitive to changes in bond length and basis set compared to the polarizability values since the hyperpolarizability is a quartic term, so these differences are unsurprising. A similar comparison can be made with the quadrupole and hexadecapole moments. Our quadrupole moment results were in extremely good agreement with literature values, while there was relatively poor agreement between all hexadecapole moments (Table 4.12). The hexadecapole moment, similar to the hyperpolarizability, is more difficult than the quadrupole moment to calculate as its magnitude is quite small (the atomic units are ea_0^4) and is therefore more sensitive to differences in the methods used to calculate it.

Table 4.10: Comparison between our polarizability results and other theoretical values. All values listed were calculated at the CCSD(T) level of theory. Our results were calculated at a maximum field strength of 0.01 au.

Data	Bond Length (Å)	Basis Set	α_{xx}	α_{zz}
This work	1.159 95	ACCT	12.6673	26.6950
	1.159 95	ACCQ	12.7747	26.6171
	1.159 95	APC3	12.7714	26.6001
Maroulis [20]	1.1600	DU1	12.98	27.04
Maroulis [20]	1.1600	DU3	12.99	27.07
Haskopoulos [11]	1.1600	7s5p4d2f	12.8966	26.8184
Kalugina [15]	1.1283	aug-cc-pV5Z	12.92	27.11

Table 4.11: Comparison between our hyperpolarizability results and other theoretical values. All values listed were calculated at the CCSD(T) level of theory. Our results were calculated at maximum field strength of 0.01 au.

Data	Bond Length (Å)	Basis Set	γ_{xxxx}	γ_{xxzz}	γ_{zzzz}
This work	1.159 95	ACCT	728	375	953
	1.159 95	ACCQ	852	448	1073
	1.159 95	APC3	1039	532	1255
Maroulis [20]	1.1600	DU1	1040	554	1297
Maroulis [20]	1.1600	DU3	1085	591	1349
Haskopoulos [11]	1.1600	7s5p4d2f	1023	547	1312

Table 4.12: Comparison between our quadrupole moment and hexadecapole moment results and other theoretical values. All values listed were calculated at the CCSD(T) level of theory, except for the results by Kalugina, which were calculated with (R)CCSD(T).

Data	Bond Length (Å)	Basis Set	θ	ϕ
This work	1.159 95	ACCT	−3.195	−3.07
	1.159 95	ACCQ	−3.173	−2.36
	1.159 95	APC3	−3.176	−2.53
Maroulis [20]	1.1600	DU1	−3.19	−1.6
Maroulis [20]	1.1600	DU3	−3.19	−1.7
Haskopoulos [11]	1.1600	7s5p4d2f	−3.201	−3.12
Kalugina [15]	1.1283	aug-cc-pV5Z	−3.15	−2.08

4.5.2 Comparison with Experiment

We also compared our results with experimental values. The experimental values use the isotropic polarizability and hyperpolarizability, the equations for which are listed below (Eq. 4.4 and Eq. 4.5 [11]).

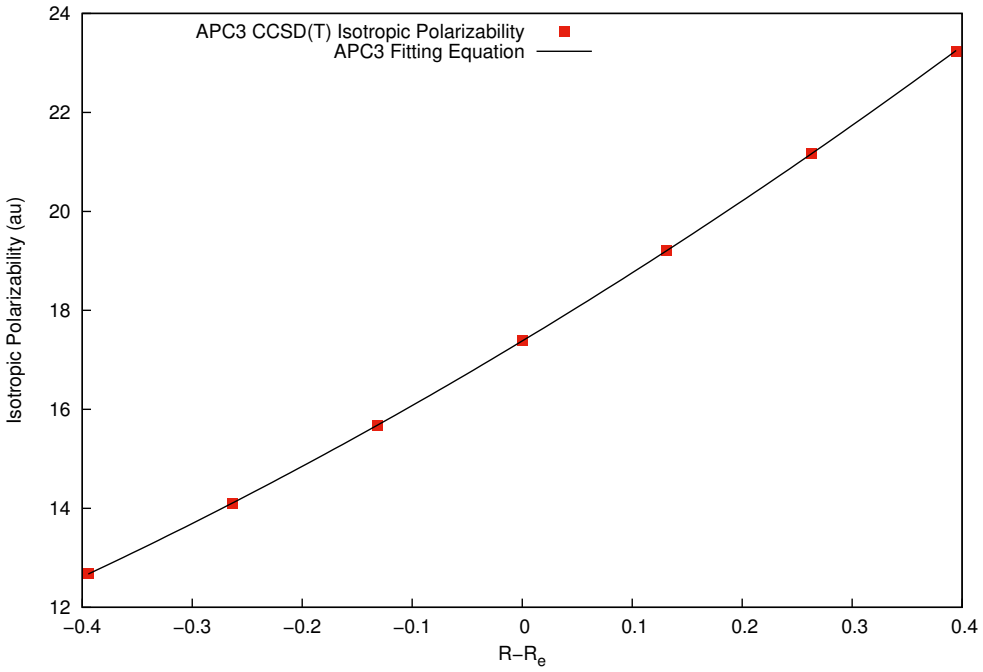
$$\bar{\alpha} = \frac{\alpha_{zz} + 2\alpha_{xx}}{3} \tag{4.4}$$

$$\bar{\gamma} = \frac{3\gamma_{zzzz} + 8\gamma_{xxxx} + 12\gamma_{xxzz}}{15} \tag{4.5}$$

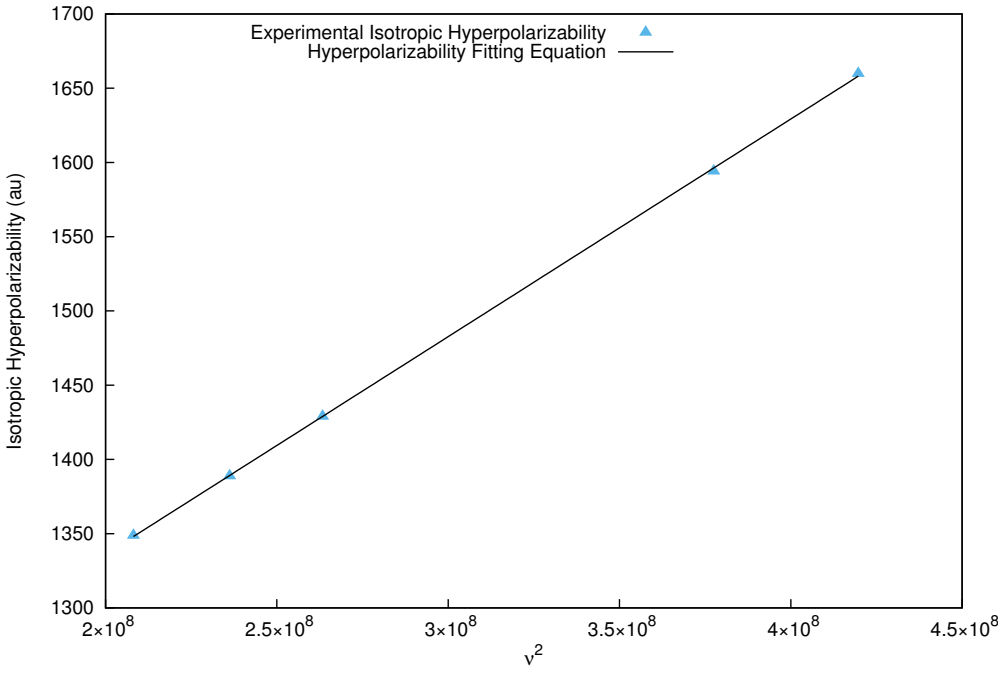
The experimental polarizability values were found from the overtone Raman spectrum of carbon dioxide, taken by Tejeda *et al.* [33]. They found the derivative of the isotropic polarizability with respect to symmetry coordinates; to compare our results, we fit our isotropic polarizabilities against the difference in bond length from equilibrium (Figure 4.6a) and converted the derivative to symmetry coordinates. As listed in Table 4.13, our polarizability results were within reasonable agreement with experiment, although our value was about 0.7 au lower than the experimental value. This difference could be due to vibrational contributions to the polarizability, although these contributions are thought to be small [11].

The coefficients of our theoretical isotropic polarizability fits were compared with fitting coefficients by Maroulis [20]. Although their fitting equation, which was fit to theoretical results, included up to the fourth power, the coefficients of the linear and quadratic terms are in good agreement. A similar analysis was carried out for fits to the isotropic hyperpolarizability versus $R - R_e$, with good agreement with the APC3 basis set. The results of these fits are listed in Table 4.14.

The experimental hyperpolarizability results were obtained by D. P. Shelton [31] using ESHG (electronic second harmonic generation) at various frequencies. For CO_2, the ESHG hyperpolarizability was found to have little vibrational contribution [31]. To compare the experimental and theoretical values, the experimental isotropic hyperpolarizability was plotted against the squared frequency, as shown in Figure 4.6b. The function was then



(a) Polarizability Calculation



(b) Hyperpolarizability Extrapolation

Figure 4.6: a) The fit used to derive the theoretical isotropic polarizability derivative that is compared to literature. The values used are the APC3 CCSD(T) results at a maximum field strength of 0.01 au. b) The fit used to extrapolate the isotropic hyperpolarizability at zero frequency from experimental values.

Table 4.13: Comparison between experimental results and our theoretical results. The theoretical values were calculated at the CCSD(T) level of theory at a maximum field strength of 0.01 au. The polarizability results are the derivative of the isotropic polarizability with respect to the symmetry coordinates. The experimental isotropic hyperpolarizability value was obtained from ESHG results and extrapolated to zero frequency.

Data	Polarizability ($\frac{\delta\bar{\alpha}}{\delta S_1}$)	Hyperpolarizability ($\bar{\gamma}$)
This work (ACCT)	9.4264	879.0017
This work (ACCQ)	9.4666	1027.6244
This work (APC3)	9.4797	1231.2587
Tejeda [33]	10.1101 ± 0.0642	
Shelton [31]		1043.0029

Table 4.14: Comparison of fitting coefficients for the isotropic polarizability and hyperpolarizability. Our equation included up to the quadratic term while the equation from Maroulis including up to the quartic term.

Property	Data	A	B
Polarizability	This work (ACCT)	13.33	3.65
	This work (ACCQ)	13.39	3.68
	This work (APC3)	13.41	3.73
	Maroulis [20]	13.81	3.78
Hyperpolarizability	This work (ACCT)	969	764
	This work (ACCQ)	1190	930
	This work (APC3)	1435	822
	Maroulis [20]	1493	1041

used to extrapolate the hyperpolarizability at zero field. Our isotropic hyperpolarizabilities, specifically the ACCQ calculated value at 1027 au, are in quite good agreement with experiment. The results of the comparison are shown in Table 4.13.

Chapter 5

Dimer Results

With the results from the CO_2 monomer, the interaction-induced dipole moment of a carbon dioxide dimer can be calculated using the procedure described in Section 3.3. The dimer configuration used was the T-shaped geometry, shown in Figure 5.1. Of the possible dimer configurations, this geometry will likely have one of the largest induced dipole moments, as the slightly positively-charged carbon atom of the second molecule can interact directly with the slightly negatively-charged oxygen on the first molecule.

5.1 Computational Details

The following results for the T-shaped dimer were obtained using the GAMESS *ab initio* software package [29, 8, 26]. The C-C distance (r) of the dimer was increased from 3.0 Å to 15.0 Å in increments of 0.5 Å. The C-O bond length used was 1.15995 Å. For the RHF and MP2 levels of theory, used with the ACCT, ACCQ, and APC3 basis sets, the dipole moments can be obtained directly from the calculations. The CCSD and CCSD(T) results, used with the ACCT basis set, require the use of a finite-field approach to calculate the dipole moments. An electric field from -0.005 to 0.005 au in increments of 0.001 au was used, and the dimer was placed in the electric field with Molecule 1 parallel to the electric field.

The fits of these energies versus the electric field are shown in Figure 5.2, where Figure 5.2a is when the C-C distance is 3.0 Å, and Figure 5.2b is when the C-C distance is 15.0 Å.

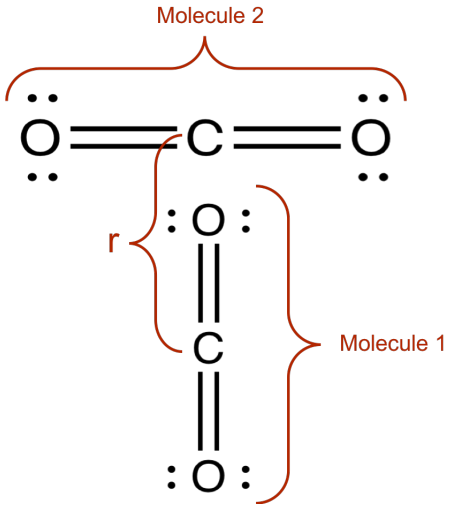
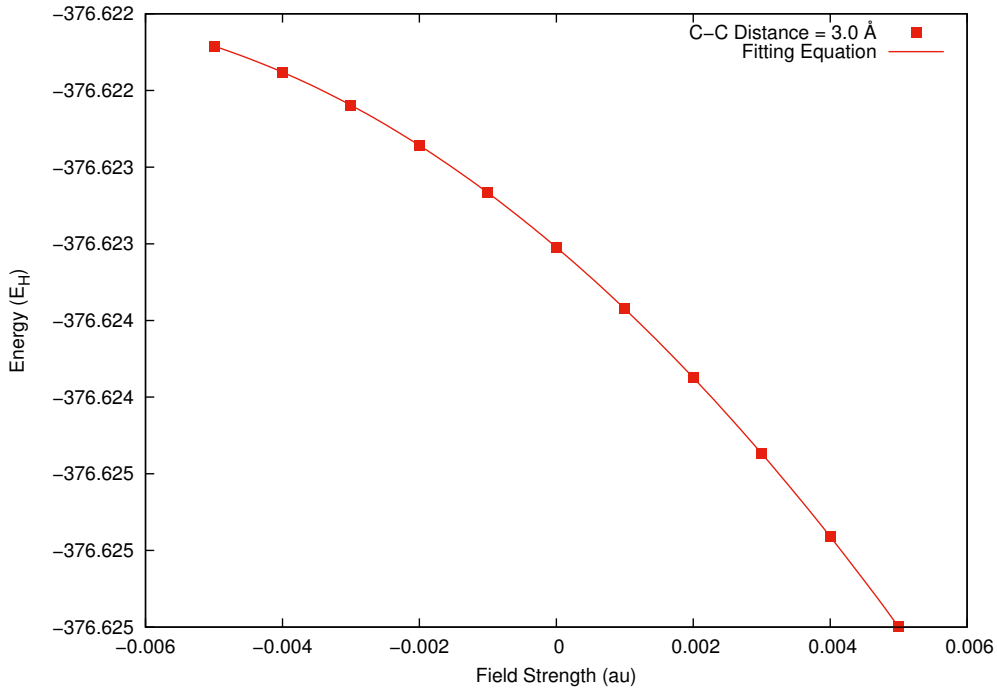
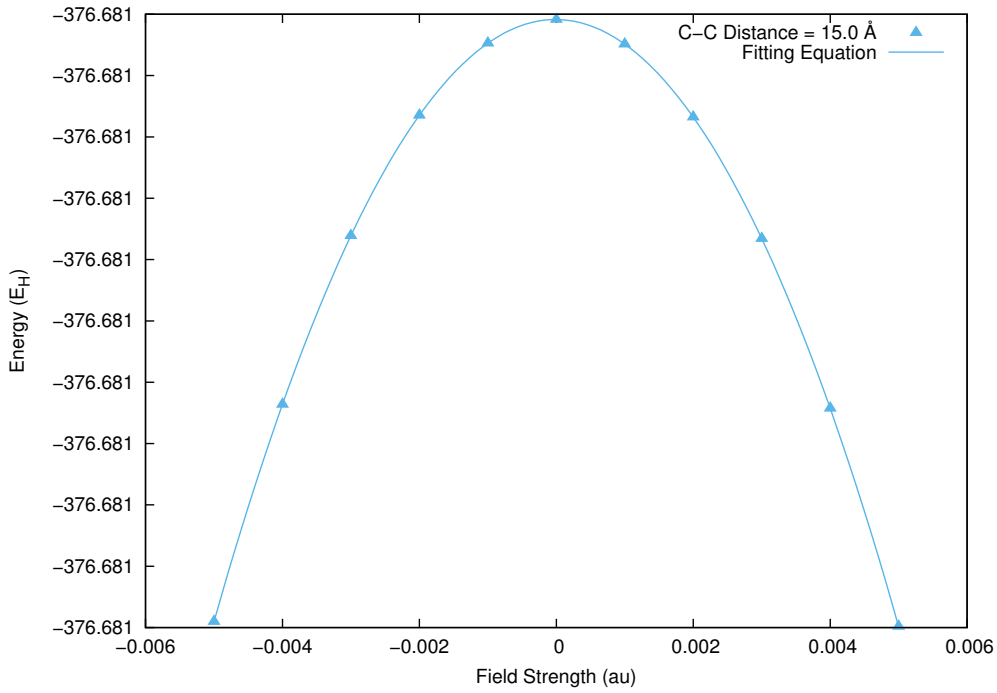


Figure 5.1: The T-shaped CO_2 dimer used in this work.



(a) C-C Distance of 3.0 Å



(b) C-C Distance of 15.0 Å

Figure 5.2: The energies of the carbon dioxide dimer versus electric field. The short-range distance is very asymmetric, while the long-range distance is close to parabolic.

As the C-C distance increases, the shape of the plots become increasingly symmetric. The complete set of energies are listed in Appendix C.1. The negative first derivative of these fits were taken, and the value of the derivative when the field is zero is the dipole moment that was used. All results were counterpoise corrected.

5.2 Results

5.2.1 Calculated Dipole Moments

The dipole moments obtained from the *ab initio* results are listed in Tables 5.1 and 5.2. At the smallest C-C distance, the dipole moment is very large; as the C-C distance increases, the dipole moment decreases and approaches zero. This is expected since the molecules in the dimer will interact less the further away they become. For all basis sets and levels of theory, the dipole moment exhibited relatively large changes in magnitude until the interatomic C-C distance reached 6.0 Å, at which point the change in the dipole moment from the previous distance was less than 0.005 au.

For the results using the ACCT basis set, the RHF values were the largest in magnitude, while the CCSD(T) results were the smallest. However, the difference between the levels of theory were small, especially at the larger C-C distances. The differences between the basis sets were also minimal, with the ACCQ and APC3 basis sets giving nearly identical results for the RHF and MP2 levels of theory. However, as we currently do not have ACCQ or APC3 coupled-cluster results to compare to, more work is needed to determine which basis sets are sufficient for the dimer calculations.

5.2.2 Fitting Results

The calculated dipole moments for each basis set and level of theory were plotted against r (in atomic units) then fit to a function. These functions were then compared to the literature equation, Eq. 3.16 [5, 23]. The form of the fitting function was similar to that of the literature function. Both the fitting function and the literature function consist of two $B_{\lambda_1\lambda_2\Lambda L}$ terms, which measure the effect of the isotropic averaged polarizability of one molecule on the

Table 5.1: The calculated *ab initio* interaction-induced dipole moments of a CO_2 dimer for the ACCT basis set at the RHF, MP2, CCSD, and CCSD(T) levels of theory.

r		ACCT			
Å	au	RHF	MP2	CCSD	CCSD(T)
3.0	5.6692	-0.4089	-0.3780	-0.3826	-0.3765
3.5	6.6140	-0.1874	-0.1744	-0.1748	-0.1730
4.0	7.5589	-0.1014	-0.0946	-0.0935	-0.0923
4.5	8.5038	-0.0600	-0.0559	-0.0547	-0.0538
5.0	9.4486	-0.0379	-0.0353	-0.0348	-0.0341
5.5	10.3935	-0.0252	-0.0234	-0.0234	-0.0229
6.0	11.3384	-0.0175	-0.0162	-0.0164	-0.0160
6.5	12.2832	-0.0125	-0.0116	-0.0117	-0.0115
7.0	13.2281	-9.22×10^{-3}	-8.56×10^{-3}	-8.70×10^{-3}	-8.50×10^{-3}
7.5	14.1729	-6.95×10^{-3}	-6.45×10^{-3}	-6.59×10^{-3}	-6.45×10^{-3}
8.0	15.1178	-5.34×10^{-3}	-4.96×10^{-3}	-5.07×10^{-3}	-4.96×10^{-3}
8.5	16.0627	-4.17×10^{-3}	-3.87×10^{-3}	-3.96×10^{-3}	-3.87×10^{-3}
9.0	17.0075	-3.31×10^{-3}	-3.07×10^{-3}	-3.13×10^{-3}	-3.06×10^{-3}
9.5	17.9524	-2.66×10^{-3}	-2.47×10^{-3}	-2.51×10^{-3}	-2.45×10^{-3}
10.0	18.8973	-2.16×10^{-3}	-2.01×10^{-3}	-2.03×10^{-3}	-1.99×10^{-3}
10.5	19.8421	-1.77×10^{-3}	-1.65×10^{-3}	-1.67×10^{-3}	-1.63×10^{-3}
11.0	20.7870	-1.47×10^{-3}	-1.36×10^{-3}	-1.38×10^{-3}	-1.35×10^{-3}
11.5	21.7319	-1.23×10^{-3}	-1.14×10^{-3}	-1.15×10^{-3}	-1.13×10^{-3}
12.0	22.6767	-1.04×10^{-3}	-9.61×10^{-4}	-9.71×10^{-4}	-9.49×10^{-4}
12.5	23.6216	-8.79×10^{-4}	-8.16×10^{-4}	-8.24×10^{-4}	-8.05×10^{-4}
13.0	24.5664	-7.51×10^{-4}	-6.98×10^{-4}	-7.04×10^{-4}	-6.88×10^{-4}
13.5	25.5113	-6.45×10^{-4}	-5.98×10^{-4}	-6.05×10^{-4}	-5.91×10^{-4}
14.0	26.4562	-5.57×10^{-4}	-5.17×10^{-4}	-5.23×10^{-4}	-5.10×10^{-4}
14.5	27.4010	-4.84×10^{-4}	-4.49×10^{-4}	-4.54×10^{-4}	-4.46×10^{-4}
15.0	28.3459	-4.22×10^{-4}	-3.92×10^{-4}	-3.99×10^{-4}	-3.89×10^{-4}

Table 5.2: The calculated *ab initio* interaction-induced dipole moments of a CO_2 dimer for the ACCQ and APC3 basis sets at the RHF and MP2 levels of theory.

r		ACCQ		APC3	
Å	au	RHF	MP2	RHF	MP2
3.0	5.6692	-0.4094	-0.3782	-0.4095	-0.3777
3.5	6.6140	-0.1875	-0.1743	-0.1875	-0.1739
4.0	7.5589	-0.1015	-0.0945	-0.1015	-0.0943
4.5	8.5038	-0.0599	-0.0557	-0.0600	-0.0557
5.0	9.4486	-0.0378	-0.0351	-0.0378	-0.0351
5.5	10.3935	-0.0251	-0.0233	-0.0251	-0.0233
6.0	11.3384	-0.0174	-0.0161	-0.0174	-0.0161
6.5	12.2832	-0.0125	-0.0116	-0.0125	-0.0116
7.0	13.2281	-9.20×10^{-3}	-8.52×10^{-3}	-9.21×10^{-3}	-8.52×10^{-3}
7.5	14.1729	-6.93×10^{-3}	-6.42×10^{-3}	-6.94×10^{-3}	-6.42×10^{-3}
8.0	15.1178	-5.33×10^{-3}	-4.93×10^{-3}	-5.33×10^{-3}	-4.93×10^{-3}
8.5	16.0627	-4.16×10^{-3}	-3.86×10^{-3}	-4.17×10^{-3}	-3.85×10^{-3}
9.0	17.0075	-3.30×10^{-3}	-3.06×10^{-3}	-3.30×10^{-3}	-3.06×10^{-3}
9.5	17.9524	-2.65×10^{-3}	-2.46×10^{-3}	-2.65×10^{-3}	-2.46×10^{-3}
10.0	18.8973	-2.16×10^{-3}	-2.00×10^{-3}	-2.16×10^{-3}	-2.00×10^{-3}
10.5	19.8421	-1.77×10^{-3}	-1.64×10^{-3}	-1.77×10^{-3}	-1.64×10^{-3}
11.0	20.7870	-1.47×10^{-3}	-1.36×10^{-3}	-1.47×10^{-3}	-1.36×10^{-3}
11.5	21.7319	-1.23×10^{-3}	-1.14×10^{-3}	-1.23×10^{-3}	-1.14×10^{-3}
12.0	22.6767	-1.03×10^{-3}	-9.58×10^{-4}	-1.03×10^{-3}	-9.57×10^{-4}
12.5	23.6216	-8.78×10^{-4}	-8.13×10^{-4}	-8.78×10^{-4}	-8.12×10^{-4}
13.0	24.5664	-7.49×10^{-4}	-6.94×10^{-4}	-7.49×10^{-4}	-6.94×10^{-4}
13.5	25.5113	-6.43×10^{-4}	-5.96×10^{-4}	-6.44×10^{-4}	-5.96×10^{-4}
14.0	26.4562	-5.57×10^{-4}	-5.16×10^{-4}	-5.57×10^{-4}	-5.15×10^{-4}
14.5	27.4010	-4.83×10^{-4}	-4.47×10^{-4}	-4.84×10^{-4}	-4.47×10^{-4}
15.0	28.3459	-4.22×10^{-4}	-3.91×10^{-4}	-4.22×10^{-4}	-3.91×10^{-4}

quadrupole and hexadecapole moment of the other, followed by two exponential functions, as shown in Eq. 5.1. The $B_{\lambda_1\lambda_2\Lambda L}$ terms describe the dipole moments in the long-range region well (Figure 5.3), and the exponential portions contribute to a better fit in both the long-range and short-range region. The derivation of these equations is described in Section 3.3.

$$\begin{aligned}\mu_0(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = &-\frac{281.138}{r^4} - \frac{129.468}{r^6} \\ &- 0.304\exp(-\frac{r - 7.0562}{1.342}) - 0.0264\exp(-\frac{r - 7.0562}{0.561})\end{aligned} \tag{3.16}$$

$$\mu_{actual}(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = -\frac{3\sqrt{3}\,B_{2023}}{2\,r^4} + \frac{5\sqrt{5}\,B_{4045}}{8\,r^6} - a\,\exp(b\,r) - c\,\exp(d\,r) \tag{5.1}$$

$$B_{2023} = \sqrt{3}\,\alpha\,\theta \tag{5.2a}$$

$$B_{4045} = \sqrt{5}\,\alpha\,\phi \tag{5.2b}$$

The values obtained in Chapter 4 that were used in the $B_{\lambda_1\lambda_2\Lambda L}$ portion of the fitting functions are listed below in Table 5.3. This portion corresponds to the approximate induction model that was discussed previously. To find the exponential portion of the equation, which is usually found by fitting the induction model to experimental data, the $B_{\lambda_1\lambda_2\Lambda L}$ terms were subtracted from the *ab initio* dipole moments (Eqs. 5.3a, 5.3b, 5.3c). This removes the contributions from the induction portion of the function from the induced dipole moment, leaving only the exponential portions. The natural log of this equation was taken, then a linear function was fit to the resulting values (Eq. 5.3d). This first exponential function describes the long-range portion of the dipole moments where the C-C distance is large. The long-range function was then subtracted from the remaining values, leaving only

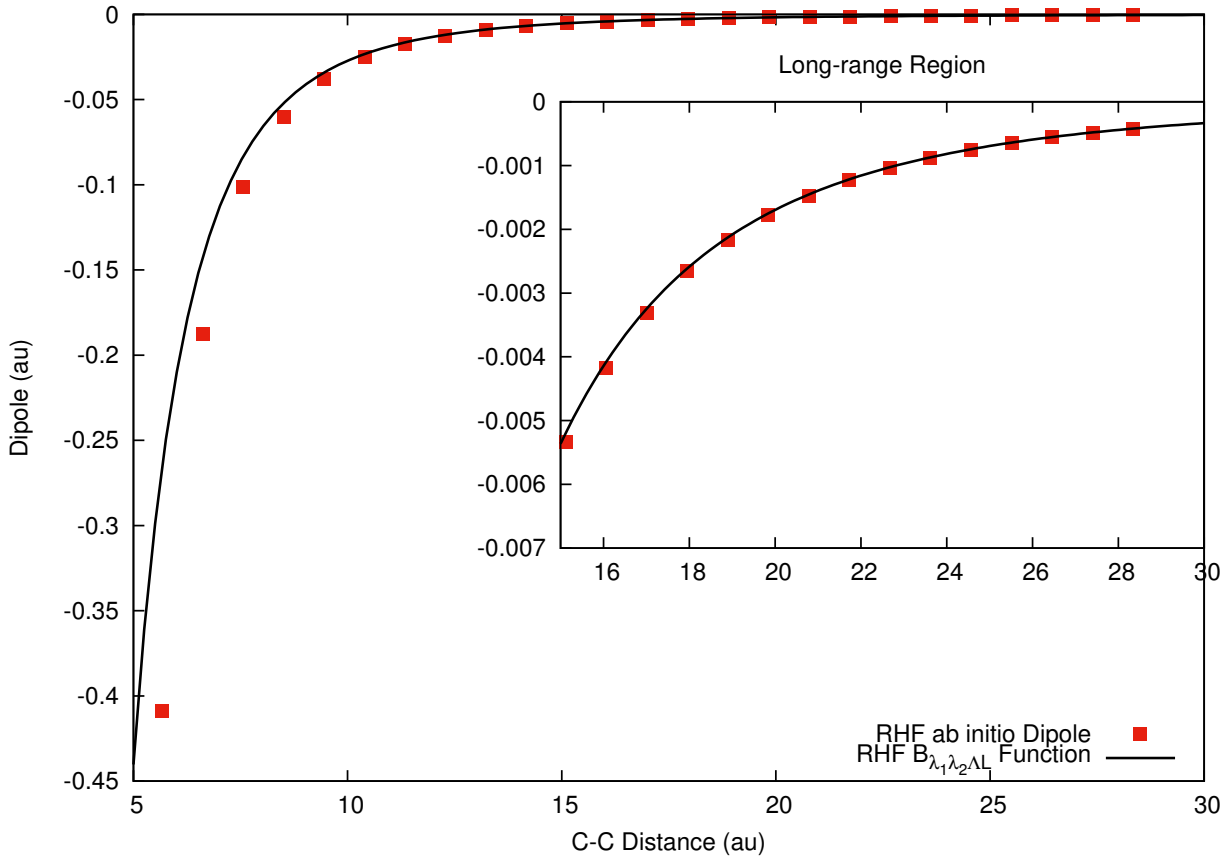


Figure 5.3: The fit of only the $B_{\lambda_1\lambda_2\Lambda L}$ values compared to the *ab initio* dipole moments for the ACCT dipole moments calculated at the RHF level of theory. The fit is close in the long-range region, but deviates in the short-range region.

Table 5.3: The ACCT, ACCQ, and APC3 values used. These were calculated for a CO_2 molecule at the equilibrium bond length.

Basis Set	Property	RHF	MP2	CCSD	CCSD(T)
ACCT	$\bar{\alpha}$	15.76	17.65	17.11	17.34
	θ	-3.82	-3.09	-3.30	-3.19
	ϕ	-2.05	-3.01	-2.79	-3.07
	B_{2023}	104.34	94.53	97.93	95.97
	B_{4045}	72.36	118.89	106.80	118.96
ACCQ	$\bar{\alpha}$	15.84	17.73	17.15	17.39
	θ	-3.80	-3.07	-3.29	-3.17
	ϕ	-1.23	-2.229	-2.06	-2.36
	B_{2023}	104.21	94.17	97.58	95.57
	B_{4045}	43.57	90.95	79.07	91.66
APC3	$\bar{\alpha}$	15.85	17.73	17.14	17.38
	θ	-3.80	-3.07	-3.29	-3.18
	ϕ	-1.23	-2.45	-2.21	-2.53
	B_{2023}	104.27	94.18	97.59	95.60
	B_{4045}	46.78	97.01	98.17	84.63

the short-range contributions to the dipole moment. The natural log of both sides was taken, and a linear function was then fit to this short-range portion (Eq. 5.3e).

$$\mu_{actual}(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) = -\frac{3\sqrt{3}\,B_{2023}}{2\,r^4} + \frac{5\sqrt{5}\,B_{4045}}{8\,r^6} - a\,\exp(b\,r) - c\,\exp(d\,r) \tag{5.3a}$$

$$\Delta\mu = \mu_{actual}(r, r_1, r_2, \Omega_1, \Omega_2, \Omega) + \frac{3\sqrt{3}\,B_{2023}}{2\,r^4} - \frac{5\sqrt{5}\,B_{4045}}{8\,r^6} \tag{5.3b}$$

$$\Delta\mu = -a\,\exp(b\,r) - c\,\exp(d\,r) \tag{5.3c}$$

$$\ln(\Delta\mu) = d\,r + \ln(c) \tag{5.3d}$$

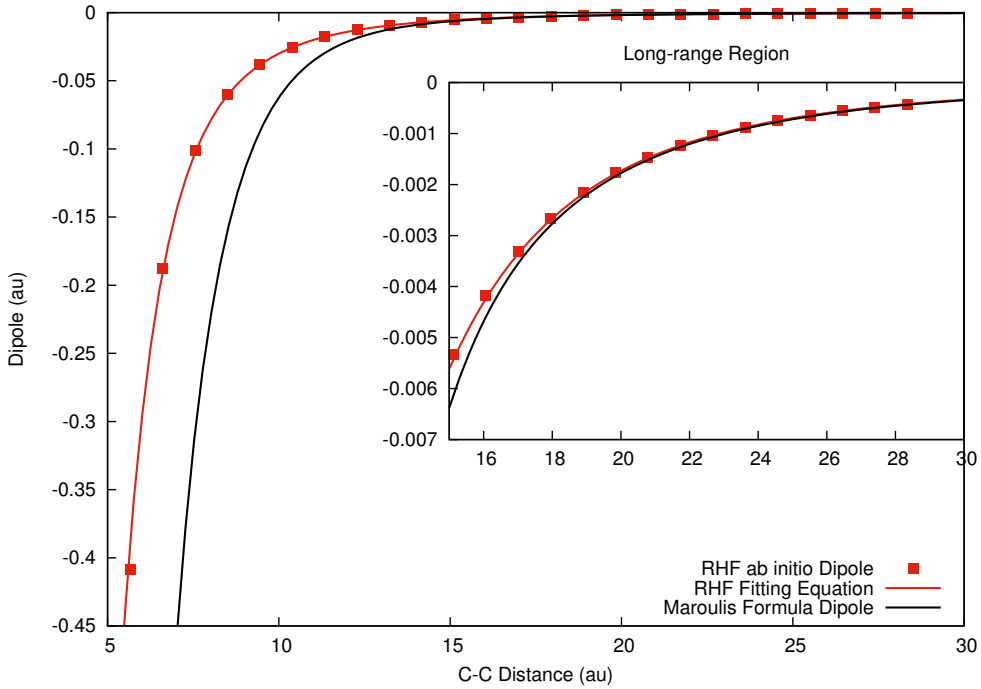
$$\ln(\Delta\mu - c\,\exp(d\,r)) = b\,r + \ln(a) \tag{5.3e}$$

The division between the short- and long-range points, called the breakpoint which was included in the fits for both the short-range and long-range regions, was tested by using 14.0-15.0 Å as the long-range and 3.5-14.0 Å as the short-range points. This was then moved iteratively, containing more points in the long-range and less in the short-range, until the long-range points included 4.5-15.0 Å, and the short-range included 3.5-4.5 Å. The root mean squared error, maximum error, and percent error were calculated for each breakpoint. The complete set of fitting parameters and errors are listed in Appendix C.2. The first point, a distance of 3.0 Å, was not used for the fitting as the potential energy is large and thus this dimer is unlikely to occur in a low-temperature environment.

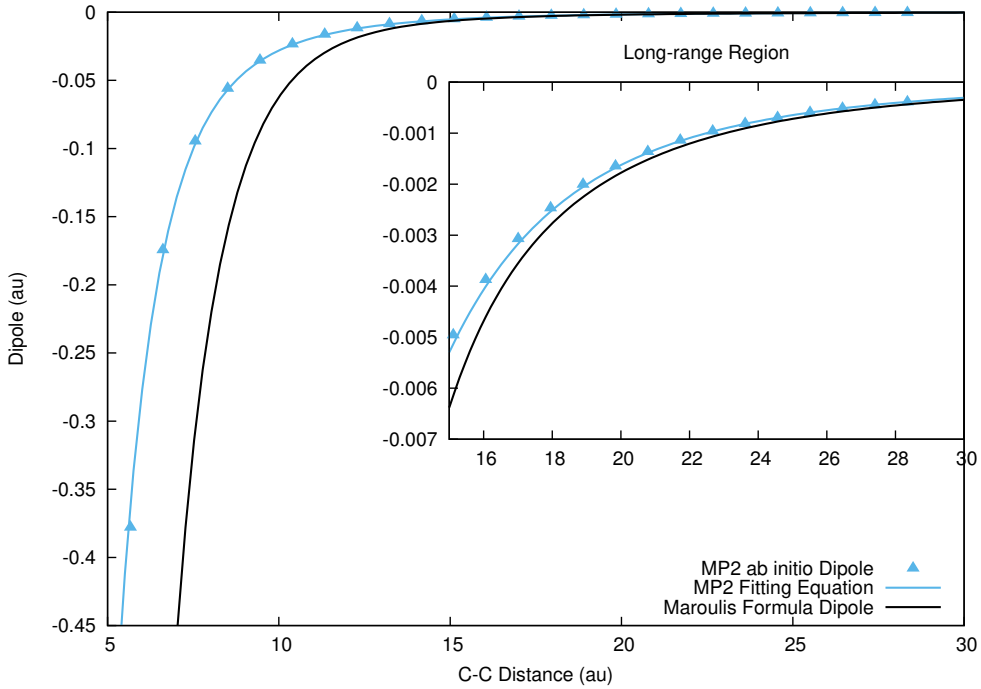
For the RHF fitting results, all three basis sets used had the smallest root mean squared error when the breakpoint was at 4.5 Å. At the MP2 level of theory, the ACCT results had the smallest error at the 4.5 Å breakpoint, while the ACCQ and APC3 results were at the 5.0 Å breakpoint. For the CCSD and CCSD(T) results, the breakpoint was at 5.0 Å. The fitting coefficients and the root mean squared errors are listed in Table 5.4. As seen in Figure 5.4, the functions obtained from the ACCT basis set fit the *ab initio* dipole moments closely, especially in the long-range region when compared to the function derived from literature. As the C-C distance of the dimer increases, the interaction-induced dipole moment approaches zero; this is expected since the molecules in the dimer should interact less with each other as the distance increases.

Table 5.4: The fitting coefficients for the breakpoint with the smallest root mean squared error.

Basis Set	Level of Theory	a	b	c	d	RMSE
ACCT	RHF	49.010	-1.074	0.085	-0.389	8.57E-05
	MP2	35.367	-1.018	0.0471	-0.314	1.17E-04
	CCSD	103.070	-1.192	0.0572	-0.368	7.83E-05
	CCSD(T)	120.550	-1.212	0.0724	-0.391	1.57E-04
ACCQ	RHF	49.069	-1.074	0.081	-0.389	7.86E-05
	MP2	29.352	-0.986	0.031	-0.297	9.01E-05
APC3	RHF	48.415	-1.072	0.082	-0.390	7.97E-05
	MP2	28.457	-0.982	0.032	-0.297	9.79E-05

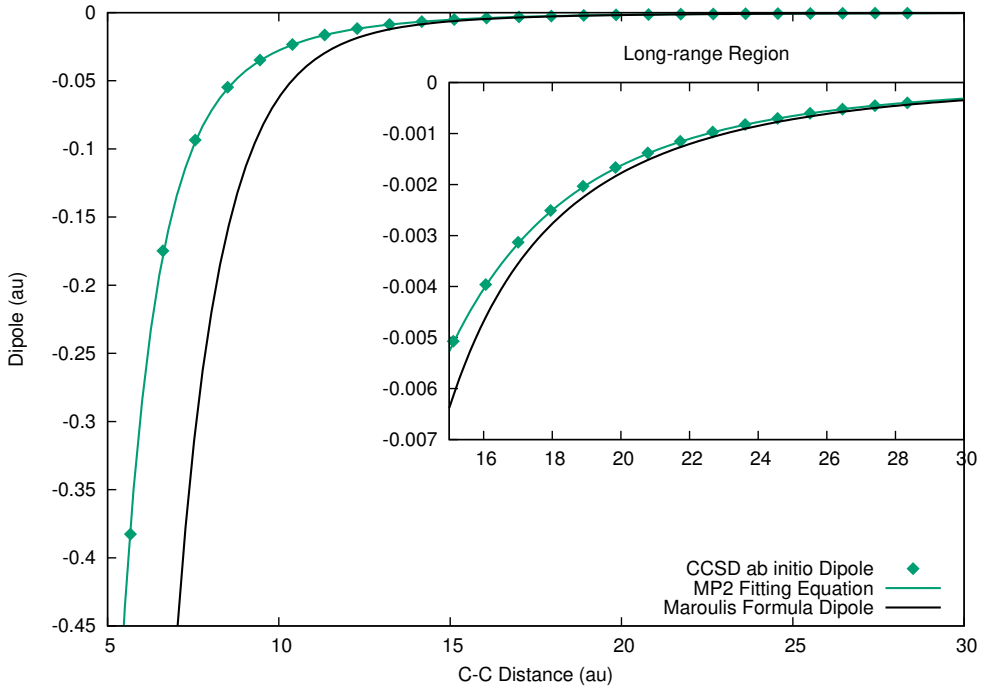


(a) RHF Fitting Results

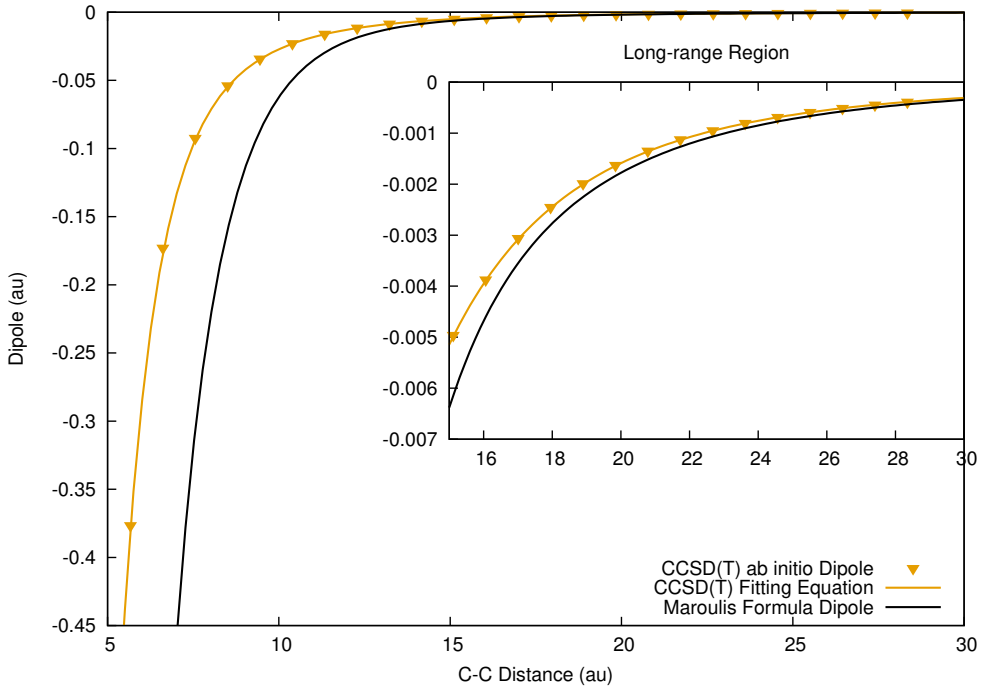


(b) MP2 Fitting Results

Figure 5.4: The ACCT *ab initio* dipole moments compared to the fitting results and the literature fitting equation.



(c) CCSD Fitting Results



(d) CCSD(T) Fitting Results

Figure 5.4: The ACCT *ab initio* dipole moments compared to the fitting results and the literature fitting equation (continued).

Although the root mean squared error of the ACCT results at the RHF level is smaller than that of the CCSD(T) level, the difference between the residuals of the RHF results as a whole is greater than that of the CCSD(T) results. Figure 5.5 shows that at a C-C distance of 7.5 Å, the CCSD(T) residuals are close to zero; at a C-C distance of 11.0 Å, where the interaction between the components of the dimer is small, the errors of all levels of theory are comparable and approach zero. The maximum errors for all levels of theory and basis sets were on the order of 10^{-4}, which is quite small, indicating that the fitting functions we calculated are a very good description of the *ab initio* interaction-induced dipole moments. The results for the ACCQ and APC3 basis sets are similar, and the complete set of results is listed in Appendix C.3.

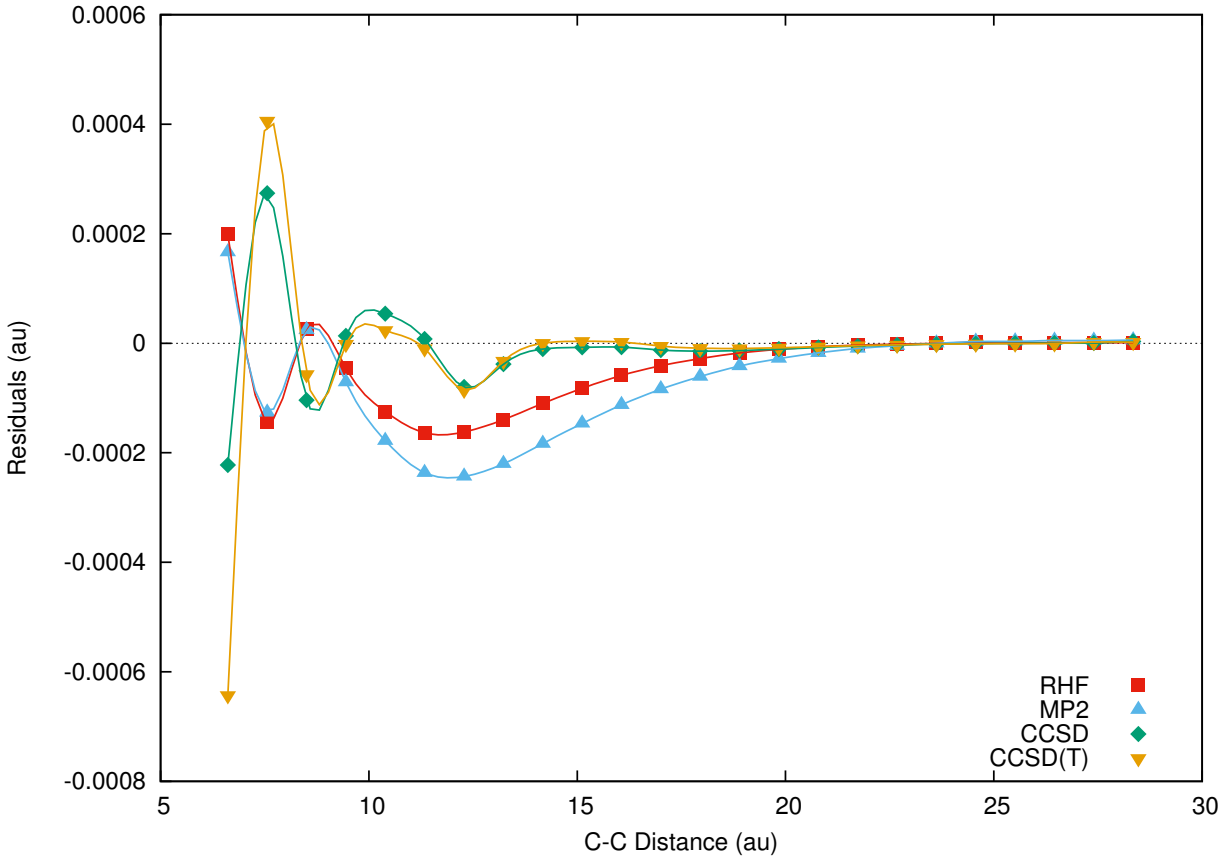


Figure 5.5: The difference between the *ab initio* dipole moments and the fitting equation for the ACCT CO_2 dimer results.

Chapter 6

Conclusions

6.1 Summary of Results

6.1.1 CO_2 Monomer Results

We were able to calculate accurate polarizability and hyperpolarizability values for a carbon dioxide monomer. The ACCT, ACCQ, and APC3 basis sets were found to be the best choices for these calculations. The bond length dependence was also investigated, along with the effect of the field strength on the results. Table 6.1 summarizes the results found for this chapter. The values are from the CCSD(T) level of theory with a maximum field strength of 0.01 au and at the equilibrium bond length of 1.15995 Å. These values were used in Chapter 5 to calculate the interaction-induced dipole moment of a carbon dioxide dimer.

Table 6.1: A complete set of response properties calculated at the CCSD(T) level of theory for a carbon dioxide molecule at the equilibrium bond length.

Property	ACCT	ACCQ	APC3
θ	-3.19	-3.17	-3.18
ϕ	-3.07	-2.36	-2.53
α_{xx}	12.67	12.77	12.77
α_{zz}	26.70	26.62	26.60
γ_{zzzz}	953.37	1073.25	1255.27
γ_{xxxx}	728.39	852.49	1039.30
γ_{xxzz}	494.10	587.84	703.48

6.1.2 CO_2 Dimer Results

For the interaction-induced dipole moments of a T-shaped CO_2 dimer, we have developed fitting equations for the RHF and MP2 levels of theory using the ACCT, ACCQ, and APC3 basis sets. Fitting equations for the CCSD and CCSD(T) levels of theory were also calculated for the ACCT basis set. Across all basis sets and levels of theory used, the largest root mean squared error was 1.66×10^{-4} for the RHF results with the ACCQ basis set. The fitting equation for the ACCT basis set at the CCSD(T) level of theory is listed below as Eq. 6.1.

$$\begin{aligned}\mu_{actual}(R, r_1, r_2, \Omega_1, \Omega_2, \Omega) = &-\frac{3\sqrt{3}\,(95.97)}{2\,r^4} + \frac{5\sqrt{5}\,(118.96)}{8\,r^6} \\ &- 120.550\,\exp(-1.212\,r) - 0.0724\,\exp(-0.391\,r)\end{aligned} \tag{6.1}$$

6.2 Future Work

Although the work done in the above chapters has provided accurate results and fitting equations, further investigations can and should be done. The response properties have been calculated for the symmetric stretch of carbon dioxide, but we have not yet calculated the effect of the asymmetric stretch. For the carbon dioxide dimer, more work at higher levels of theory and basis sets will be done. The calculations for the CCSD and CCSD(T) levels of theory at the ACCQ basis set are in progress, and the calculations for the APC3 basis set will also be performed. Should the APC3 basis set prove to be too computationally intensive, other comparable basis sets will be investigated. This work only investigated the T-shaped dimer; other dimer configurations will be used as well.

6.3 Conclusions

In conclusion, we have, to the best of our knowledge, reported the first purely *ab initio* interaction-induced dipole moment model for a carbon dioxide dimer. After further investigation, these results will be used in molecular dynamics simulations to calculate CIA.

The *ab initio* CIA model can then be used to compare to current models and can help achieve better calculations of the paleoclimate of ancient Mars.

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Appendices

A Additional Data

A.1 Complete Field Energies

Table A.1: The results for the field strength calculations for the RHF and MP2 levels of theory using the ACCT basis set. The bond length is 1.15995 Å.

	RHF			MP2		
Field Strength	X	XZ	Z	X	XZ	Z
0.000	−187.709 518	−187.709 518	−187.709 518	−188.321 230	−188.321 230	−188.321 230
0.001	−187.709 523	−187.709 527	−187.709 530	−188.321 236	−188.321 240	−188.321 244
0.002	−187.709 540	−187.709 553	−187.709 565	−188.321 253	−188.321 269	−188.321 285
0.003	−187.709 568	−187.709 596	−187.709 624	−188.321 281	−188.321 317	−188.321 353
0.004	−187.709 607	−187.709 657	−187.709 707	−188.321 321	−188.321 385	−188.321 449
0.005	−187.709 656	−187.709 735	−187.709 814	−188.321 372	−188.321 472	−188.321 572
0.006	−187.709 718	−187.709 831	−187.709 944	−188.321 434	−188.321 578	−188.321 723
0.007	−187.709 790	−187.709 944	−187.710 097	−188.321 508	−188.321 704	−188.321 901
0.008	−187.709 873	−187.710 074	−187.710 275	−188.321 593	−188.321 849	−188.322 106
0.009	−187.709 967	−187.710 222	−187.710 476	−188.321 689	−188.322 014	−188.322 339
0.010	−187.710 073	−187.710 387	−187.710 701	−188.321 797	−188.322 198	−188.322 599
0.015	−187.710 767	−187.711 474	−187.712 181	−188.322 506	−188.323 409	−188.324 312
0.020	−187.711 739	−187.712 996	−187.714 254	−188.323 500	−188.325 105	−188.326 711
0.025	−187.712 992	−187.714 956	−187.716 922	−188.324 780	−188.327 289	−188.329 800
0.030	−187.714 526	−187.717 354	−187.720 187	−188.326 348	−188.329 962	−188.333 582
0.035	−187.716 342	−187.720 194	−187.724 052	−188.328 205	−188.333 126	−188.338 060
0.040	−187.718 443	−187.723 476	−187.728 520	−188.330 353	−188.336 785	−188.343 239
0.045	−187.720 832	−187.727 204	−187.733 595	−188.332 796	−188.340 942	−188.349 125
0.050	−187.723 511	−187.731 383	−187.739 282	−188.335 537	−188.345 602	−188.355 725
0.055	−187.726 484	−187.736 015	−187.745 587	−188.338 578	−188.350 771	−188.363 050
0.060	−187.729 755	−187.741 106	−187.752 517	−188.341 926	−188.356 453	−188.371 109
0.065	−187.733 329	−187.746 663	−187.760 080	−188.345 584	−188.362 659	−188.379 918
0.070	−187.737 210	−187.752 692	−187.768 286	−188.349 560	−188.369 397	−188.389 495
0.075	−187.741 405	−187.759 205	−187.777 148	−188.353 859	−188.376 680	−188.399 861
0.080	−187.745 922	−187.766 214	−187.786 682	−188.358 490	−188.384 527	−188.411 049
0.090	−187.755 956	−187.781 806	−187.807 848	−188.368 789	−188.402 027	−188.436 072
0.100	−187.767 406	−187.799 851	−187.832 042	−188.380 564	−188.422 428	−188.465 261

A.2 Exact γ_{xxzz} vs. Calculated γ_{xxzz}

Table A.2: The ACCD calculated energies and the γ_{xxzz} values and errors for a carbon dioxide molecule in the xz-direction. The bond length is 1.15995 Å.

Field Strength	Energy	γ_{xxzz}	Percent Error
0.0025	−187.662 886	230.7371	8.090
0.0050	−187.663 050	213.9355	0.219
0.0075	−187.663 323	214.3638	0.420
0.0100	−187.663 705	214.5351	0.500
0.0125	−187.664 196	215.0638	0.748
0.0150	−187.664 797	215.7208	1.056
0.0175	−187.665 507	216.5032	1.422
0.0200	−187.666 327	217.4251	1.854
0.0225	−187.667 256	218.4818	2.349
0.0250	−187.668 296	219.6797	2.910
0.0275	−187.669 446	221.0228	3.539
0.0300	−187.670 706	222.5173	4.240
0.0350	−187.673 559	225.9813	5.862
0.0400	−187.676 858	230.1332	7.807
0.0450	−187.680 606	235.0554	10.113
0.0500	−187.684 807	240.8504	12.828
0.0550	−187.689 466	247.6577	16.017
0.0600	−187.694 588	255.6614	19.766

Table A.3: The ACCT calculated energies and the γ_{xxzz} values and errors for a carbon dioxide molecule in the xz-direction. The bond length is 1.15995 Å.

Field Strength	Energy	γ_{xxzz}	Percent Error
0.0025	−187.709 573	263.1224	1.286
0.0050	−187.709 739	262.4779	1.038
0.0075	−187.710 017	260.8419	0.408
0.0100	−187.710 405	261.3573	0.607
0.0125	−187.710 904	262.1670	0.918
0.0150	−187.711 514	263.1410	1.293
0.0175	−187.712 236	264.3456	1.757
0.0200	−187.713 069	265.7473	2.296
0.0225	−187.714 014	267.3688	2.921
0.0250	−187.715 070	269.2152	3.631
0.0275	−187.716 240	271.2990	4.434
0.0300	−187.717 521	273.6279	5.330
0.0350	−187.720 424	279.0901	7.433
0.0400	−187.723 781	285.7561	9.999
0.0450	−187.727 599	293.8380	13.110
0.0500	−187.731 881	303.6301	16.879
0.0550	−187.736 634	315.5519	21.468
0.0600	−187.741 868	330.2193	27.114

A.3 Basis Set Analysis Full Results

Table A.4: The complete set of results for the α_{xx} values for all basis sets tested. These were obtained from the Hartree-Fock level of theory with an equilibrium bond length of 1.15995 Å.

Percent from Equilibrium	CCD	CCT	CCQ	ACCD	ACCT	ACCQ	DACCD	DACCT	PC3	APC3	APC4
-20.0	5.80	7.47	8.32	8.69	9.08	9.16	9.16	9.18	8.83	9.17	9.17
-19.0	5.87	7.56	8.43	8.81	9.21	9.29	9.29	9.31	8.95	9.30	9.31
-18.0	5.94	7.65	8.54	8.94	9.34	9.42	9.42	9.45	9.07	9.43	9.44
-17.0	6.02	7.75	8.65	9.06	9.47	9.56	9.56	9.58	9.20	9.57	9.58
-16.0	6.09	7.84	8.77	9.19	9.61	9.69	9.70	9.72	9.32	9.70	9.71
-15.0	6.16	7.94	8.88	9.31	9.74	9.83	9.83	9.86	9.45	9.84	9.85
-14.0	6.23	8.03	8.99	9.44	9.88	9.97	9.97	9.99	9.57	9.98	9.99
-13.0	6.30	8.13	9.10	9.57	10.01	10.11	10.11	10.13	9.70	10.12	10.13
-12.0	6.37	8.22	9.22	9.70	10.15	10.25	10.25	10.27	9.82	10.26	10.26
-11.0	6.44	8.32	9.33	9.83	10.28	10.38	10.39	10.41	9.95	10.40	10.40
-10.0	6.51	8.41	9.44	9.96	10.42	10.52	10.53	10.55	10.08	10.54	10.54
-9.0	6.58	8.51	9.56	10.08	10.56	10.66	10.67	10.69	10.21	10.68	10.69
-8.0	6.65	8.60	9.67	10.21	10.70	10.81	10.81	10.83	10.33	10.82	10.83
-7.0	6.72	8.70	9.78	10.35	10.84	10.95	10.95	10.98	10.46	10.96	10.97
-6.0	6.79	8.79	9.89	10.48	10.97	11.09	11.10	11.12	10.59	11.10	11.11
-5.0	6.86	8.89	10.01	10.61	11.11	11.23	11.24	11.26	10.72	11.24	11.25
-4.0	6.92	8.98	10.12	10.74	11.25	11.37	11.38	11.40	10.84	11.38	11.40
-3.0	6.99	9.07	10.23	10.87	11.39	11.51	11.53	11.55	10.97	11.53	11.54
-2.0	7.05	9.16	10.34	11.00	11.53	11.66	11.67	11.69	11.10	11.67	11.68
-1.0	7.12	9.26	10.46	11.13	11.67	11.80	11.81	11.83	11.22	11.81	11.82
0.0	7.18	9.35	10.57	11.26	11.81	11.94	11.95	11.97	11.35	11.95	11.97
1.0	7.24	9.44	10.68	11.40	11.95	12.08	12.10	12.12	11.48	12.10	12.11
2.0	7.31	9.53	10.79	11.53	12.08	12.22	12.24	12.26	11.60	12.24	12.25
3.0	7.37	9.61	10.90	11.66	12.22	12.36	12.38	12.40	11.73	12.38	12.39
4.0	7.42	9.70	11.01	11.79	12.36	12.50	12.52	12.54	11.85	12.52	12.53
5.0	7.48	9.79	11.11	11.92	12.50	12.64	12.66	12.68	11.98	12.66	12.67
6.0	7.54	9.87	11.22	12.05	12.63	12.78	12.80	12.83	12.10	12.80	12.82
7.0	7.60	9.95	11.33	12.17	12.77	12.92	12.94	12.97	12.22	12.94	12.96
8.0	7.65	10.04	11.43	12.30	12.91	13.06	13.08	13.11	12.34	13.08	13.09
9.0	7.70	10.12	11.54	12.43	13.04	13.20	13.22	13.24	12.47	13.22	13.23
10.0	7.76	10.20	11.64	12.55	13.18	13.34	13.36	13.38	12.59	13.36	13.37
11.0	7.81	10.27	11.74	12.68	13.31	13.47	13.49	13.52	12.71	13.49	13.51
12.0	7.86	10.35	11.84	12.80	13.44	13.61	13.63	13.66	12.82	13.63	13.65
13.0	7.90	10.43	11.94	12.93	13.57	13.74	13.76	13.79	12.94	13.77	13.78
14.0	7.95	10.50	12.04	13.05	13.70	13.88	13.90	13.93	13.06	13.90	13.92
15.0	8.00	10.57	12.13	13.17	13.83	14.01	14.03	14.06	13.17	14.03	14.05
16.0	8.04	10.64	12.23	13.29	13.96	14.14	14.16	14.19	13.28	14.17	14.18
17.0	8.09	10.71	12.32	13.41	14.09	14.27	14.29	14.32	13.40	14.30	14.31
18.0	8.13	10.77	12.41	13.52	14.21	14.40	14.42	14.45	13.51	14.43	14.44
19.0	8.17	10.84	12.50	13.64	14.34	14.53	14.55	14.58	13.62	14.55	14.57
20.0	8.21	10.90	12.59	13.75	14.46	14.65	14.67	14.71	13.72	14.68	14.70

Table A.5: The complete set of results for the α_{zz} values for all basis sets tested. These were obtained from the Hartree-Fock level of theory with an equilibrium bond length of 1.15995 Å.

Percent from Equilibrium	CCD	CCT	CCQ	ACCD	ACCT	ACCQ	DACCD	DACCT	PC3	APC3	APC4
-20.00	12.74	14.52	15.33	15.91	15.83	15.83	16.00	15.86	15.81	15.83	15.84
-19.00	13.05	14.82	15.64	16.24	16.15	16.16	16.32	16.18	16.14	16.15	16.16
-18.00	13.37	15.13	15.96	16.57	16.48	16.49	16.64	16.51	16.47	16.48	16.49
-17.00	13.69	15.44	16.29	16.90	16.82	16.82	16.97	16.85	16.81	16.82	16.83
-16.00	14.02	15.77	16.62	17.25	17.16	17.17	17.32	17.19	17.15	17.17	17.17
-15.00	14.35	16.10	16.96	17.60	17.52	17.52	17.66	17.55	17.50	17.52	17.52
-14.00	14.69	16.44	17.31	17.96	17.88	17.88	18.02	17.91	17.86	17.88	17.88
-13.00	15.04	16.79	17.67	18.32	18.25	18.25	18.38	18.27	18.23	18.25	18.25
-12.00	15.40	17.14	18.03	18.70	18.62	18.63	18.75	18.65	18.61	18.62	18.63
-11.00	15.76	17.50	18.40	19.08	19.01	19.01	19.12	19.03	18.99	19.01	19.01
-10.00	16.12	17.87	18.77	19.46	19.40	19.40	19.50	19.42	19.38	19.39	19.40
-9.00	16.49	18.25	19.15	19.85	19.79	19.79	19.89	19.81	19.78	19.79	19.79
-8.00	16.87	18.63	19.54	20.25	20.20	20.20	20.28	20.22	20.18	20.19	20.20
-7.00	17.26	19.02	19.94	20.65	20.61	20.61	20.69	20.63	20.59	20.60	20.61
-6.00	17.65	19.41	20.34	21.07	21.02	21.02	21.09	21.04	21.00	21.02	21.02
-5.00	18.04	19.81	20.75	21.48	21.45	21.44	21.51	21.47	21.43	21.44	21.44
-4.00	18.44	20.22	21.16	21.90	21.88	21.87	21.93	21.90	21.86	21.87	21.87
-3.00	18.85	20.64	21.58	22.33	22.31	22.31	22.35	22.33	22.29	22.30	22.31
-2.00	19.26	21.06	22.01	22.76	22.75	22.75	22.78	22.77	22.73	22.75	22.75
-1.00	19.68	21.48	22.44	23.20	23.20	23.20	23.22	23.22	23.18	23.19	23.20
0.00	20.10	21.91	22.88	23.65	23.66	23.65	23.66	23.67	23.63	23.65	23.65
1.00	20.52	22.34	23.32	24.09	24.11	24.11	24.11	24.13	24.09	24.10	24.11
2.00	20.95	22.78	23.77	24.55	24.58	24.57	24.57	24.60	24.55	24.57	24.57
3.00	21.38	23.23	24.23	25.01	25.05	25.04	25.02	25.07	25.02	25.04	25.04
4.00	21.82	23.68	24.69	25.47	25.52	25.52	25.49	25.54	25.50	25.51	25.51
5.00	22.26	24.13	25.15	25.94	26.00	25.99	25.96	26.02	25.98	25.99	25.99
6.00	22.71	24.59	25.62	26.41	26.48	26.48	26.43	26.50	26.46	26.47	26.47
7.00	23.16	25.05	26.09	26.88	26.97	26.97	26.91	26.99	26.95	26.96	26.96
8.00	23.61	25.52	26.57	27.36	27.46	27.46	27.39	27.48	27.44	27.45	27.45
9.00	24.07	25.98	27.05	27.85	27.96	27.95	27.88	27.98	27.93	27.95	27.95
10.00	24.53	26.46	27.53	28.33	28.46	28.46	28.37	28.48	28.43	28.45	28.45
11.00	24.99	26.93	28.02	28.82	28.96	28.96	28.86	28.99	28.93	28.95	28.95
12.00	25.46	27.41	28.51	29.32	29.47	29.47	29.36	29.50	29.44	29.46	29.46
13.00	25.93	27.89	29.00	29.82	29.98	29.98	29.86	30.01	29.95	29.97	29.97
14.00	26.40	28.38	29.50	30.32	30.50	30.50	30.37	30.52	30.47	30.48	30.49
15.00	26.88	28.87	30.00	30.82	31.01	31.01	30.88	31.04	30.98	31.00	31.01
16.00	27.35	29.36	30.51	31.33	31.54	31.54	31.40	31.57	31.51	31.53	31.53
17.00	27.84	29.86	31.01	31.84	32.06	32.06	31.92	32.10	32.03	32.05	32.06
18.00	28.32	30.36	31.53	32.36	32.59	32.60	32.44	32.63	32.56	32.58	32.59
19.00	28.81	30.86	32.04	32.88	33.13	33.13	32.97	33.16	33.10	33.12	33.13
20.00	29.30	31.37	32.56	33.41	33.67	33.67	33.50	33.71	33.63	33.66	33.67

Table A.6: The complete set of results for the γ_{xxxx} values for all basis sets tested. These were obtained from the Hartree-Fock level of theory with an equilibrium bond length of 1.15995 Å.

Percent from Equilibrium	CCD	CCT	CCQ	ACCD	ACCT	ACCQ	DACCD	DACCT	PC3	APC3	APC4
-20.00	30.63	67.99	123.06	215.72	292.92	354.43	389.50	412.90	212.98	418.04	419.99
-19.00	31.96	70.54	126.93	222.45	301.55	364.45	399.87	424.80	219.06	430.10	432.14
-18.00	33.29	73.17	130.96	229.57	310.60	374.94	410.70	437.25	225.43	442.72	444.84
-17.00	34.61	75.89	135.13	237.06	320.05	385.88	422.00	450.22	232.09	455.90	458.07
-16.00	35.92	78.67	139.45	244.92	329.90	397.27	433.76	463.73	239.03	469.62	471.85
-15.00	37.21	81.51	143.89	253.15	340.14	409.10	445.99	477.77	246.25	483.89	486.16
-14.00	38.47	84.40	148.44	261.74	350.76	421.37	458.68	492.32	253.73	498.70	500.99
-13.00	39.70	87.34	153.10	270.67	361.74	434.06	471.83	507.38	261.47	514.04	516.34
-12.00	40.90	90.31	157.86	279.95	373.09	447.18	485.43	522.95	269.44	529.91	532.21
-11.00	42.05	93.31	162.70	289.55	384.79	460.70	499.49	539.01	277.66	546.30	548.58
-10.00	43.16	96.34	167.62	299.48	396.84	474.64	513.99	555.56	286.09	563.19	565.45
-9.00	44.22	99.37	172.60	309.71	409.22	488.98	528.94	572.60	294.74	580.59	582.81
-8.00	45.23	102.41	177.64	320.25	421.93	503.70	544.32	590.10	303.60	598.47	600.65
-7.00	46.18	105.44	182.72	331.07	434.96	518.81	560.14	608.07	312.66	616.84	618.96
-6.00	47.07	108.46	187.83	342.17	448.31	534.30	576.39	626.49	321.90	635.68	637.75
-5.00	47.90	111.46	192.98	353.54	461.96	550.15	593.05	645.36	331.33	654.99	656.98
-4.00	48.67	114.43	198.14	365.16	475.91	566.36	610.13	664.66	340.93	674.74	676.67
-3.00	49.37	117.36	203.31	377.03	490.14	582.91	627.62	684.38	350.70	694.94	696.78
-2.00	50.01	120.25	208.47	389.12	504.66	599.80	645.50	704.51	360.63	715.57	717.32
-1.00	50.58	123.07	213.63	401.43	519.44	617.01	663.77	725.04	370.71	736.61	738.28
0.00	51.08	125.84	218.77	413.94	534.48	634.54	682.42	745.96	380.92	758.06	759.63
1.00	51.52	128.53	223.87	426.65	549.77	652.36	701.44	767.26	391.28	779.91	781.37
2.00	51.89	131.14	228.95	439.53	565.30	670.47	720.82	788.91	401.76	802.13	803.49
3.00	52.19	133.67	233.97	452.58	581.07	688.85	740.54	810.91	412.35	824.73	825.97
4.00	52.43	136.09	238.95	465.79	597.05	707.49	760.60	833.25	423.05	847.67	848.79
5.00	52.60	138.41	243.86	479.14	613.24	726.38	780.98	855.90	433.85	870.96	871.95
6.00	52.70	140.62	248.70	492.61	629.62	745.50	801.68	878.85	444.73	894.57	895.43
7.00	52.74	142.71	253.47	506.21	646.19	764.84	822.67	902.08	455.69	918.50	919.21
8.00	52.71	144.67	258.15	519.91	662.93	784.38	843.95	925.59	466.71	942.72	943.28
9.00	52.63	146.50	262.74	533.70	679.83	804.11	865.50	949.35	477.78	967.21	967.63
10.00	52.48	148.19	267.24	547.58	696.88	824.01	887.31	973.35	488.90	991.97	992.22
11.00	52.26	149.74	271.63	561.54	714.06	844.07	909.35	997.56	500.04	1016.98	1017.06
12.00	51.99	151.14	275.92	575.55	731.36	864.27	931.62	1021.97	511.20	1042.22	1042.12
13.00	51.66	152.40	280.08	589.62	748.77	884.59	954.10	1046.57	522.37	1067.66	1067.38
14.00	51.27	153.49	284.13	603.73	766.27	905.02	976.77	1071.32	533.52	1093.30	1092.89
15.00	50.82	154.44	288.04	617.87	783.84	925.54	999.62	1096.23	544.66	1119.11	1118.51
16.00	50.32	155.22	291.82	632.03	801.48	946.14	1022.62	1121.26	555.76	1145.08	1144.28
17.00	49.76	155.85	295.47	646.20	819.16	966.80	1045.76	1146.40	566.82	1171.19	1170.18
18.00	49.14	156.32	298.96	660.37	836.87	987.49	1069.02	1171.62	577.82	1197.41	1196.18
19.00	48.47	156.64	302.31	674.54	854.60	1008.21	1092.37	1196.91	588.75	1223.73	1222.28
20.00	47.75	156.80	305.51	688.68	872.33	1028.94	1115.80	1222.25	599.60	1250.12	1248.45

Table A.7: The complete set of results for the γ_{zzzz} values for all basis sets tested. These were obtained from the Hartree-Fock level of theory with an equilibrium bond length of 1.15995 Å.

Percent from Equilibrium	CCD	CCT	CCQ	ACCD	ACCT	ACCQ	DACCD	DACCT	PC3	APC3	APC4
-20.00	-30.60	46.74	226.61	458.08	564.73	633.51	724.80	675.00	538.82	690.25	685.81
-19.00	-33.68	43.16	223.52	461.08	570.13	639.56	732.56	681.58	541.03	697.55	692.75
-18.00	-36.92	39.48	220.29	464.25	575.72	645.85	740.55	688.43	543.28	705.08	699.95
-17.00	-40.32	35.69	216.91	467.57	581.48	652.37	748.75	695.53	545.57	712.82	707.40
-16.00	-43.90	31.78	213.41	471.04	587.39	659.10	757.16	702.88	547.88	720.75	715.08
-15.00	-47.66	27.74	209.77	474.65	593.44	666.04	765.77	710.46	550.19	728.87	722.99
-14.00	-51.61	23.57	206.01	478.40	599.62	673.18	774.57	718.25	552.49	737.16	731.11
-13.00	-55.77	19.25	202.12	482.29	605.91	680.50	783.56	726.25	554.78	745.63	739.43
-12.00	-60.12	14.77	198.13	486.32	612.31	687.99	792.74	734.45	557.04	754.26	747.96
-11.00	-64.69	10.12	194.02	490.49	618.81	695.66	802.13	742.83	559.26	763.06	756.68
-10.00	-69.47	5.31	189.81	494.79	625.41	703.50	811.71	751.40	561.45	772.02	765.60
-9.00	-74.47	0.30	185.50	499.25	632.11	711.52	821.51	760.16	563.59	781.15	774.71
-8.00	-79.68	-4.89	181.10	503.86	638.91	719.70	831.53	769.11	565.69	790.45	784.02
-7.00	-85.11	-10.27	176.61	508.63	645.80	728.06	841.79	778.25	567.75	799.94	793.53
-6.00	-90.75	-15.84	172.05	513.57	652.80	736.60	852.29	787.59	569.78	809.62	803.26
-5.00	-96.60	-21.59	167.42	518.70	659.91	745.33	863.07	797.14	571.78	819.50	813.21
-4.00	-102.65	-27.53	162.72	524.04	667.14	754.26	874.14	806.93	573.78	829.61	823.39
-3.00	-108.89	-33.65	157.98	529.60	674.51	763.41	885.54	816.96	575.78	839.96	833.83
-2.00	-115.30	-39.92	153.20	535.40	682.05	772.79	897.28	827.27	577.81	850.58	844.56
-1.00	-121.87	-46.33	148.41	541.49	689.76	782.43	909.40	837.89	579.90	861.50	855.59
0.00	-128.56	-52.86	143.61	547.89	697.70	792.36	921.94	848.85	582.09	872.76	866.96
1.00	-135.37	-59.47	138.84	554.63	705.88	802.61	934.94	860.19	584.41	884.39	878.72
2.00	-142.26	-66.15	134.13	561.78	714.35	813.23	948.46	871.97	586.92	896.45	890.90
3.00	-149.19	-72.84	129.51	569.37	723.17	824.25	962.54	884.25	589.68	908.99	903.57
4.00	-156.13	-79.50	125.03	577.46	732.40	835.73	977.24	897.08	592.74	922.06	916.78
5.00	-163.03	-86.08	120.73	586.14	742.09	847.74	992.65	910.55	596.19	935.75	930.60
6.00	-169.85	-92.50	116.67	595.46	752.33	860.36	1008.83	924.73	600.11	950.14	945.11
7.00	-176.53	-98.72	112.92	605.52	763.21	873.66	1025.88	939.72	604.59	965.30	960.41
8.00	-183.02	-104.64	109.56	616.42	774.82	887.74	1043.88	955.63	609.74	981.36	976.60
9.00	-189.25	-110.17	106.67	628.26	787.28	902.71	1062.95	972.58	615.68	998.41	993.78
10.00	-195.14	-115.23	104.36	641.18	800.72	918.69	1083.21	990.69	622.55	1016.59	1012.09
11.00	-200.63	-119.71	102.74	655.29	815.27	935.83	1104.80	1010.12	630.49	1036.03	1031.66
12.00	-205.63	-123.48	101.93	670.77	831.09	954.26	1127.86	1031.02	639.66	1056.91	1052.66
13.00	-210.05	-126.43	102.08	687.77	848.36	974.17	1152.56	1053.57	650.25	1079.38	1075.25
14.00	-213.79	-128.43	103.33	706.49	867.27	995.74	1179.07	1077.97	662.45	1103.65	1099.66
15.00	-216.76	-129.32	105.87	727.12	888.03	1019.18	1207.62	1104.44	676.49	1129.93	1126.06
16.00	-218.85	-128.96	109.86	749.90	910.87	1044.71	1238.41	1133.21	692.59	1158.44	1154.68
17.00	-219.93	-127.17	115.52	775.08	936.05	1072.60	1271.69	1164.54	711.03	1189.46	1185.79
18.00	-219.89	-123.79	123.05	802.92	963.85	1103.11	1307.73	1198.72	732.09	1223.26	1219.68
19.00	-218.60	-118.63	132.68	833.72	994.57	1136.54	1346.82	1236.05	756.07	1260.14	1256.64
20.00	-215.94	-111.51	144.66	867.79	1028.54	1173.22	1389.29	1276.86	783.30	1300.44	1297.01

Table A.8: The complete set of results for the γ_{xxzz} values for all basis sets tested. These were obtained from the Hartree-Fock level of theory with an equilibrium bond length of 1.15995 Å.

Percent from Equilibrium	CCD	CCT	CCQ	ACCD	ACCT	ACCQ	DACCD	DACCT	PC3	APC3	APC4
-20.00	9.45	23.10	61.01	130.28	174.08	208.78	244.00	236.72	149.94	238.84	239.51
-19.00	10.52	23.61	61.45	132.49	176.51	211.77	247.36	240.41	152.13	242.57	243.23
-18.00	11.66	24.21	61.98	134.92	179.12	214.95	250.95	244.33	154.47	246.52	247.17
-17.00	12.88	24.90	62.59	137.56	181.92	218.33	254.78	248.48	156.95	250.71	251.34
-16.00	14.18	25.68	63.28	140.41	184.90	221.90	258.85	252.86	159.58	255.14	255.74
-15.00	15.55	26.56	64.05	143.47	188.08	225.67	263.16	257.47	162.35	259.80	260.38
-14.00	17.01	27.53	64.92	146.73	191.44	229.64	267.71	262.32	165.27	264.69	265.24
-13.00	18.54	28.60	65.87	150.20	194.99	233.80	272.51	267.39	168.33	269.81	270.34
-12.00	20.15	29.78	66.93	153.87	198.74	238.16	277.56	272.70	171.53	275.17	275.67
-11.00	21.85	31.05	68.08	157.73	202.69	242.73	282.86	278.24	174.87	280.76	281.23
-10.00	23.63	32.43	69.34	161.80	206.83	247.50	288.42	284.01	178.36	286.59	287.04
-9.00	25.50	33.91	70.70	166.07	211.17	252.47	294.22	290.02	182.01	292.66	293.08
-8.00	27.46	35.49	72.18	170.53	215.72	257.66	300.29	296.27	185.81	298.96	299.37
-7.00	29.52	37.19	73.77	175.19	220.47	263.06	306.61	302.76	189.77	305.51	305.90
-6.00	31.67	39.00	75.48	180.05	225.43	268.69	313.20	309.50	193.90	312.30	312.68
-5.00	33.92	40.92	77.32	185.11	230.61	274.53	320.04	316.49	198.20	319.34	319.71
-4.00	36.29	42.96	79.29	190.37	235.99	280.61	327.15	323.73	202.68	326.64	327.00
-3.00	38.77	45.13	81.40	195.83	241.60	286.92	334.53	331.22	207.35	334.19	334.55
-2.00	41.37	47.42	83.65	201.50	247.43	293.47	342.18	338.98	212.20	342.00	342.36
-1.00	44.10	49.85	86.05	207.38	253.49	300.27	350.11	347.00	217.25	350.08	350.44
0.00	46.96	52.41	88.61	213.47	259.78	307.32	358.32	355.30	222.50	358.43	358.80
1.00	49.98	55.13	91.32	219.78	266.32	314.62	366.81	363.87	227.96	367.06	367.44
2.00	53.16	58.00	94.21	226.31	273.10	322.19	375.60	372.74	233.63	375.97	376.36
3.00	56.51	61.04	97.27	233.08	280.14	330.04	384.69	381.90	239.52	385.18	385.58
4.00	60.04	64.25	100.51	240.08	287.44	338.17	394.09	391.37	245.64	394.70	395.11
5.00	63.77	67.65	103.96	247.34	295.03	346.60	403.81	401.15	251.99	404.53	404.95
6.00	67.73	71.25	107.60	254.85	302.90	355.33	413.85	411.26	258.59	414.68	415.12
7.00	71.91	75.06	111.47	262.63	311.07	364.37	424.24	421.72	265.43	425.17	425.63
8.00	76.35	79.10	115.56	270.70	319.55	373.75	434.99	432.53	272.55	436.02	436.48
9.00	81.07	83.39	119.90	279.07	328.36	383.47	446.11	443.71	279.94	447.23	447.71
10.00	86.08	87.93	124.50	287.74	337.52	393.56	457.61	455.29	287.63	458.82	459.31
11.00	91.41	92.76	129.37	296.75	347.04	404.03	469.53	467.27	295.62	470.82	471.32
12.00	97.09	97.89	134.53	306.11	356.94	414.90	481.87	479.68	303.94	483.24	483.75
13.00	103.15	103.34	140.01	315.83	367.25	426.19	494.66	492.55	312.60	496.10	496.62
14.00	109.62	109.14	145.82	325.95	377.99	437.92	507.93	505.90	321.63	509.43	509.94
15.00	116.52	115.30	151.97	336.48	389.18	450.13	521.70	519.75	331.05	523.27	523.78
16.00	123.90	121.87	158.51	347.45	400.85	462.85	536.00	534.14	340.88	537.62	538.15
17.00	131.78	128.85	165.44	358.89	413.03	476.09	550.87	549.11	351.15	552.54	553.09
18.00	140.20	136.28	172.79	370.83	425.75	489.90	566.33	564.68	361.89	568.05	568.61
19.00	149.19	144.19	180.59	383.29	439.04	504.31	582.43	580.90	373.12	584.20	584.76
20.00	158.80	152.60	188.87	396.32	452.95	519.35	599.20	597.80	384.88	601.01	601.59

A.4 Energies of CO_2 Used to Calculate Polarizabilities and Hyperpolarizabilities

Table A.9: The energies of CO_2 at different electric fields at the RHF level of theory for the ACCT basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.450 754	−187.626 233	−187.700 619	−187.709 518	−187.677 335	−187.620 957	−187.552 161
0.001	−187.450 758	−187.626 238	−187.700 625	−187.709 524	−187.677 341	−187.620 964	−187.552 168
0.002	−187.450 772	−187.626 253	−187.700 641	−187.709 541	−187.677 360	−187.620 984	−187.552 189
0.003	−187.450 796	−187.626 278	−187.700 669	−187.709 571	−187.677 392	−187.621 018	−187.552 225
0.004	−187.450 828	−187.626 314	−187.700 707	−187.709 612	−187.677 436	−187.621 065	−187.552 275
0.005	−187.450 870	−187.626 359	−187.700 756	−187.709 665	−187.677 493	−187.621 125	−187.552 339
0.006	−187.450 922	−187.626 415	−187.700 817	−187.709 730	−187.677 562	−187.621 199	−187.552 417
0.007	−187.450 982	−187.626 481	−187.700 888	−187.709 807	−187.677 644	−187.621 286	−187.552 509
0.008	−187.451 053	−187.626 557	−187.700 970	−187.709 896	−187.677 739	−187.621 387	−187.552 616
0.009	−187.451 132	−187.626 644	−187.701 064	−187.709 996	−187.677 847	−187.621 502	−187.552 737
0.010	−187.451 221	−187.626 740	−187.701 168	−187.710 108	−187.677 967	−187.621 629	−187.552 872
0.015	−187.451 805	−187.627 375	−187.701 855	−187.710 847	−187.678 757	−187.622 471	−187.553 762
0.020	−187.452 624	−187.628 265	−187.702 817	−187.711 883	−187.679 866	−187.623 650	−187.555 009
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.450 754	−187.626 233	−187.700 619	−187.709 518	−187.677 335	−187.620 957	−187.552 161
0.001	−187.450 760	−187.626 240	−187.700 627	−187.709 527	−187.677 344	−187.620 968	−187.552 173
0.002	−187.450 779	−187.626 261	−187.700 651	−187.709 553	−187.677 374	−187.621 000	−187.552 208
0.003	−187.450 812	−187.626 297	−187.700 691	−187.709 598	−187.677 423	−187.621 054	−187.552 266
0.004	−187.450 857	−187.626 348	−187.700 747	−187.709 660	−187.677 491	−187.621 129	−187.552 348
0.005	−187.450 915	−187.626 412	−187.700 819	−187.709 739	−187.677 579	−187.621 225	−187.552 453
0.006	−187.450 986	−187.626 492	−187.700 907	−187.709 837	−187.677 687	−187.621 343	−187.552 582
0.007	−187.451 070	−187.626 585	−187.701 011	−187.709 952	−187.677 814	−187.621 483	−187.552 734
0.008	−187.451 167	−187.626 693	−187.701 131	−187.710 085	−187.677 961	−187.621 644	−187.552 910
0.009	−187.451 277	−187.626 815	−187.701 267	−187.710 236	−187.678 127	−187.621 826	−187.553 109
0.010	−187.451 399	−187.626 952	−187.701 419	−187.710 405	−187.678 313	−187.622 030	−187.553 332
0.015	−187.452 207	−187.627 852	−187.702 420	−187.711 514	−187.679 537	−187.623 373	−187.554 796
0.020	−187.453 339	−187.629 113	−187.703 823	−187.713 069	−187.681 252	−187.625 255	−187.556 849
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.450 754	−187.626 233	−187.700 619	−187.709 518	−187.677 335	−187.620 957	−187.552 161
0.001	−187.450 762	−187.626 242	−187.700 630	−187.709 530	−187.677 348	−187.620 972	−187.552 177
0.002	−187.450 787	−187.626 270	−187.700 661	−187.709 565	−187.677 388	−187.621 016	−187.552 226
0.003	−187.450 828	−187.626 316	−187.700 714	−187.709 624	−187.677 454	−187.621 090	−187.552 308
0.004	−187.450 885	−187.626 382	−187.700 787	−187.709 707	−187.677 547	−187.621 193	−187.552 422
0.005	−187.450 960	−187.626 465	−187.700 882	−187.709 814	−187.677 666	−187.621 326	−187.552 568
0.006	−187.451 050	−187.626 568	−187.700 998	−187.709 944	−187.677 811	−187.621 488	−187.552 748
0.007	−187.451 157	−187.626 689	−187.701 134	−187.710 097	−187.677 984	−187.621 679	−187.552 960
0.008	−187.451 281	−187.626 829	−187.701 292	−187.710 275	−187.678 182	−187.621 900	−187.553 204
0.009	−187.451 421	−187.626 987	−187.701 471	−187.710 476	−187.678 407	−187.622 151	−187.553 481
0.010	−187.451 578	−187.627 164	−187.701 671	−187.710 701	−187.678 659	−187.622 431	−187.553 791
0.015	−187.452 609	−187.628 329	−187.702 986	−187.712 181	−187.680 316	−187.624 274	−187.555 830
0.020	−187.454 054	−187.629 961	−187.704 828	−187.714 254	−187.682 637	−187.626 857	−187.558 686

Table A.10: The energies of CO_2 at different electric fields at the RHF level of theory for the ACCQ basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.468 648	−187.641 886	−187.714 550	−187.722 229	−187.689 220	−187.632 293	−187.563 123
0.001	−187.468 653	−187.641 891	−187.714 556	−187.722 235	−187.689 226	−187.632 300	−187.563 130
0.002	−187.468 667	−187.641 907	−187.714 572	−187.722 253	−187.689 245	−187.632 320	−187.563 152
0.003	−187.468 690	−187.641 932	−187.714 600	−187.722 283	−187.689 277	−187.632 354	−187.563 188
0.004	−187.468 723	−187.641 968	−187.714 639	−187.722 324	−187.689 322	−187.632 402	−187.563 238
0.005	−187.468 766	−187.642 014	−187.714 689	−187.722 378	−187.689 380	−187.632 463	−187.563 303
0.006	−187.468 818	−187.642 071	−187.714 750	−187.722 444	−187.689 450	−187.632 538	−187.563 382
0.007	−187.468 879	−187.642 137	−187.714 822	−187.722 521	−187.689 533	−187.632 626	−187.563 476
0.008	−187.468 950	−187.642 214	−187.714 905	−187.722 611	−187.689 629	−187.632 728	−187.563 584
0.009	−187.469 030	−187.642 301	−187.714 999	−187.722 713	−187.689 738	−187.632 844	−187.563 706
0.010	−187.469 119	−187.642 399	−187.715 105	−187.722 826	−187.689 859	−187.632 974	−187.563 843
0.015	−187.469 709	−187.643 040	−187.715 799	−187.723 573	−187.690 660	−187.633 826	−187.564 745
0.020	−187.470 535	−187.643 938	−187.716 771	−187.724 621	−187.691 782	−187.635 020	−187.566 009
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.468 648	−187.641 886	−187.714 550	−187.722 229	−187.689 220	−187.632 293	−187.563 123
0.001	−187.468 654	−187.641 893	−187.714 558	−187.722 238	−187.689 230	−187.632 304	−187.563 135
0.002	−187.468 674	−187.641 915	−187.714 582	−187.722 264	−187.689 259	−187.632 336	−187.563 170
0.003	−187.468 706	−187.641 951	−187.714 622	−187.722 309	−187.689 308	−187.632 390	−187.563 229
0.004	−187.468 752	−187.642 002	−187.714 679	−187.722 371	−187.689 377	−187.632 465	−187.563 311
0.005	−187.468 810	−187.642 067	−187.714 751	−187.722 451	−187.689 465	−187.632 562	−187.563 417
0.006	−187.468 881	−187.642 146	−187.714 839	−187.722 549	−187.689 573	−187.632 681	−187.563 546
0.007	−187.468 965	−187.642 240	−187.714 943	−187.722 665	−187.689 701	−187.632 821	−187.563 699
0.008	−187.469 063	−187.642 348	−187.715 064	−187.722 798	−187.689 848	−187.632 982	−187.563 875
0.009	−187.469 173	−187.642 471	−187.715 200	−187.722 950	−187.690 015	−187.633 165	−187.564 075
0.010	−187.469 296	−187.642 608	−187.715 353	−187.723 119	−187.690 202	−187.633 370	−187.564 298
0.015	−187.470 107	−187.643 511	−187.716 358	−187.724 233	−187.691 430	−187.634 718	−187.565 769
0.020	−187.471 243	−187.644 778	−187.717 766	−187.725 793	−187.693 152	−187.636 608	−187.567 831
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.468 648	−187.641 886	−187.714 550	−187.722 229	−187.689 220	−187.632 293	−187.563 123
0.001	−187.468 656	−187.641 895	−187.714 561	−187.722 241	−187.689 233	−187.632 308	−187.563 139
0.002	−187.468 681	−187.641 923	−187.714 592	−187.722 276	−187.689 273	−187.632 352	−187.563 188
0.003	−187.468 722	−187.641 970	−187.714 645	−187.722 335	−187.689 339	−187.632 425	−187.563 270
0.004	−187.468 780	−187.642 035	−187.714 718	−187.722 418	−187.689 432	−187.632 529	−187.563 384
0.005	−187.468 854	−187.642 119	−187.714 813	−187.722 525	−187.689 551	−187.632 661	−187.563 530
0.006	−187.468 945	−187.642 221	−187.714 929	−187.722 655	−187.689 697	−187.632 823	−187.563 710
0.007	−187.469 052	−187.642 343	−187.715 065	−187.722 808	−187.689 869	−187.633 015	−187.563 922
0.008	−187.469 176	−187.642 482	−187.715 223	−187.722 986	−187.690 067	−187.633 236	−187.564 166
0.009	−187.469 316	−187.642 641	−187.715 402	−187.723 187	−187.690 293	−187.633 487	−187.564 443
0.010	−187.469 473	−187.642 818	−187.715 601	−187.723 412	−187.690 544	−187.633 767	−187.564 753
0.015	−187.470 504	−187.643 983	−187.716 917	−187.724 891	−187.692 201	−187.635 610	−187.566 792
0.020	−187.471 949	−187.645 616	−187.718 759	−187.726 964	−187.694 521	−187.638 193	−187.569 650

Table A.11: The energies of CO_2 at different electric fields at the RHF level of theory for the APC3 basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.471 065	−187.644 024	−187.716 483	−187.723 987	−187.690 835	−187.633 798	−187.564 541
0.001	−187.471 070	−187.644 029	−187.716 488	−187.723 993	−187.690 842	−187.633 805	−187.564 548
0.002	−187.471 084	−187.644 045	−187.716 505	−187.724 011	−187.690 861	−187.633 825	−187.564 569
0.003	−187.471 108	−187.644 070	−187.716 533	−187.724 041	−187.690 893	−187.633 859	−187.564 606
0.004	−187.471 141	−187.644 106	−187.716 572	−187.724 083	−187.690 938	−187.633 907	−187.564 656
0.005	−187.471 183	−187.644 152	−187.716 622	−187.724 136	−187.690 995	−187.633 969	−187.564 721
0.006	−187.471 235	−187.644 209	−187.716 683	−187.724 202	−187.691 066	−187.634 044	−187.564 800
0.007	−187.471 296	−187.644 276	−187.716 755	−187.724 280	−187.691 149	−187.634 132	−187.564 894
0.008	−187.471 367	−187.644 352	−187.716 838	−187.724 370	−187.691 245	−187.634 235	−187.565 002
0.009	−187.471 447	−187.644 440	−187.716 933	−187.724 471	−187.691 354	−187.634 350	−187.565 125
0.010	−187.471 537	−187.644 537	−187.717 038	−187.724 585	−187.691 476	−187.634 480	−187.565 262
0.015	−187.472 128	−187.645 179	−187.717 733	−187.725 333	−187.692 277	−187.635 334	−187.566 166
0.020	−187.472 955	−187.646 079	−187.718 707	−187.726 383	−187.693 402	−187.636 531	−187.567 434
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.471 065	−187.644 024	−187.716 483	−187.723 987	−187.690 835	−187.633 798	−187.564 541
0.001	−187.471 072	−187.644 031	−187.716 491	−187.723 996	−187.690 845	−187.633 809	−187.564 552
0.002	−187.471 091	−187.644 053	−187.716 515	−187.724 023	−187.690 875	−187.633 841	−187.564 588
0.003	−187.471 124	−187.644 089	−187.716 555	−187.724 067	−187.690 924	−187.633 895	−187.564 646
0.004	−187.471 169	−187.644 140	−187.716 611	−187.724 129	−187.690 992	−187.633 971	−187.564 729
0.005	−187.471 227	−187.644 205	−187.716 684	−187.724 209	−187.691 081	−187.634 067	−187.564 834
0.006	−187.471 299	−187.644 284	−187.716 772	−187.724 307	−187.691 189	−187.634 186	−187.564 964
0.007	−187.471 383	−187.644 378	−187.716 876	−187.724 423	−187.691 316	−187.634 326	−187.565 117
0.008	−187.471 480	−187.644 486	−187.716 997	−187.724 557	−187.691 464	−187.634 488	−187.565 293
0.009	−187.471 590	−187.644 609	−187.717 133	−187.724 708	−187.691 631	−187.634 671	−187.565 493
0.010	−187.471 713	−187.644 747	−187.717 286	−187.724 877	−187.691 817	−187.634 876	−187.565 716
0.015	−187.472 525	−187.645 650	−187.718 291	−187.725 991	−187.693 047	−187.636 225	−187.567 188
0.020	−187.473 662	−187.646 917	−187.719 700	−187.727 553	−187.694 770	−187.638 115	−187.569 252
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−187.471 065	−187.644 024	−187.716 483	−187.723 987	−187.690 835	−187.633 798	−187.564 541
0.001	−187.471 073	−187.644 034	−187.716 493	−187.723 999	−187.690 848	−187.633 813	−187.564 557
0.002	−187.471 098	−187.644 061	−187.716 525	−187.724 034	−187.690 888	−187.633 857	−187.564 606
0.003	−187.471 139	−187.644 108	−187.716 577	−187.724 093	−187.690 954	−187.633 931	−187.564 687
0.004	−187.471 197	−187.644 173	−187.716 651	−187.724 176	−187.691 047	−187.634 034	−187.564 801
0.005	−187.471 271	−187.644 257	−187.716 746	−187.724 283	−187.691 166	−187.634 166	−187.564 948
0.006	−187.471 362	−187.644 359	−187.716 861	−187.724 413	−187.691 312	−187.634 328	−187.565 127
0.007	−187.471 469	−187.644 481	−187.716 998	−187.724 566	−187.691 484	−187.634 520	−187.565 339
0.008	−187.471 593	−187.644 620	−187.717 155	−187.724 744	−187.691 682	−187.634 741	−187.565 584
0.009	−187.471 733	−187.644 779	−187.717 334	−187.724 945	−187.691 908	−187.634 991	−187.565 861
0.010	−187.471 890	−187.644 956	−187.717 534	−187.725 170	−187.692 159	−187.635 271	−187.566 170
0.015	−187.472 921	−187.646 121	−187.718 849	−187.726 649	−187.693 815	−187.637 114	−187.568 209
0.020	−187.474 367	−187.647 754	−187.720 692	−187.728 722	−187.696 136	−187.639 697	−187.571 066

Table A.12: The energies of CO_2 at different electric fields at the MP2 level of theory for the ACCT basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.008 549	−188.199 811	−188.292 361	−188.321 230	−188.309 938	−188.273 934	−188.222 869
0.001	−188.008 554	−188.199 816	−188.292 367	−188.321 236	−188.309 945	−188.273 942	−188.222 877
0.002	−188.008 569	−188.199 833	−188.292 385	−188.321 255	−188.309 966	−188.273 964	−188.222 901
0.003	−188.008 594	−188.199 860	−188.292 415	−188.321 287	−188.310 000	−188.274 001	−188.222 940
0.004	−188.008 629	−188.199 898	−188.292 456	−188.321 332	−188.310 048	−188.274 052	−188.222 995
0.005	−188.008 674	−188.199 947	−188.292 509	−188.321 390	−188.310 110	−188.274 118	−188.223 065
0.006	−188.008 730	−188.200 008	−188.292 574	−188.321 460	−188.310 185	−188.274 199	−188.223 151
0.007	−188.008 795	−188.200 079	−188.292 651	−188.321 543	−188.310 275	−188.274 295	−188.223 253
0.008	−188.008 870	−188.200 160	−188.292 740	−188.321 639	−188.310 378	−188.274 405	−188.223 371
0.009	−188.008 956	−188.200 253	−188.292 841	−188.321 748	−188.310 495	−188.274 530	−188.223 504
0.010	−188.009 051	−188.200 357	−188.292 954	−188.321 869	−188.310 626	−188.274 670	−188.223 653
0.015	−188.009 680	−188.201 041	−188.293 695	−188.322 670	−188.311 486	−188.275 591	−188.224 634
0.020	−188.010 560	−188.201 999	−188.294 734	−188.323 792	−188.312 693	−188.276 883	−188.226 011
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.008 549	−188.199 811	−188.292 361	−188.321 230	−188.309 938	−188.273 934	−188.222 869
0.001	−188.008 556	−188.199 819	−188.292 370	−188.321 240	−188.309 949	−188.273 947	−188.222 884
0.002	−188.008 577	−188.199 842	−188.292 397	−188.321 270	−188.309 983	−188.273 985	−188.222 926
0.003	−188.008 612	−188.199 882	−188.292 441	−188.321 320	−188.310 040	−188.274 049	−188.222 998
0.004	−188.008 661	−188.199 937	−188.292 504	−188.321 391	−188.310 119	−188.274 138	−188.223 098
0.005	−188.008 725	−188.200 009	−188.292 584	−188.321 481	−188.310 221	−188.274 253	−188.223 226
0.006	−188.008 802	−188.200 096	−188.292 682	−188.321 591	−188.310 346	−188.274 394	−188.223 383
0.007	−188.008 894	−188.200 198	−188.292 798	−188.321 722	−188.310 493	−188.274 559	−188.223 569
0.008	−188.008 999	−188.200 317	−188.292 931	−188.321 873	−188.310 663	−188.274 751	−188.223 783
0.009	−188.009 119	−188.200 452	−188.293 083	−188.322 043	−188.310 856	−188.274 968	−188.224 026
0.010	−188.009 253	−188.200 602	−188.293 252	−188.322 234	−188.311 071	−188.275 210	−188.224 298
0.015	−188.010 134	−188.201 592	−188.294 367	−188.323 491	−188.312 488	−188.276 806	−188.226 085
0.020	−188.011 369	−188.202 979	−188.295 929	−188.325 253	−188.314 475	−188.279 043	−188.228 590
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.008 549	−188.199 811	−188.292 361	−188.321 230	−188.309 938	−188.273 934	−188.222 869
0.001	−188.008 558	−188.199 821	−188.292 373	−188.321 244	−188.309 954	−188.273 953	−188.222 890
0.002	−188.008 585	−188.199 852	−188.292 409	−188.321 285	−188.310 001	−188.274 007	−188.222 952
0.003	−188.008 630	−188.199 904	−188.292 468	−188.321 353	−188.310 080	−188.274 098	−188.223 056
0.004	−188.008 694	−188.199 976	−188.292 551	−188.321 449	−188.310 190	−188.274 225	−188.223 201
0.005	−188.008 775	−188.200 070	−188.292 658	−188.321 572	−188.310 332	−188.274 388	−188.223 387
0.006	−188.008 875	−188.200 184	−188.292 789	−188.321 723	−188.310 506	−188.274 588	−188.223 615
0.007	−188.008 993	−188.200 318	−188.292 944	−188.321 901	−188.310 711	−188.274 824	−188.223 885
0.008	−188.009 128	−188.200 474	−188.293 122	−188.322 106	−188.310 948	−188.275 096	−188.224 196
0.009	−188.009 282	−188.200 650	−188.293 324	−188.322 339	−188.311 216	−188.275 405	−188.224 548
0.010	−188.009 455	−188.200 846	−188.293 550	−188.322 599	−188.311 516	−188.275 750	−188.224 942
0.015	−188.010 588	−188.202 142	−188.295 038	−188.324 312	−188.313 489	−188.278 020	−188.227 534
0.020	−188.012 176	−188.203 958	−188.297 123	−188.326 711	−188.316 254	−188.281 200	−188.231 165

Table A.13: The energies of CO_2 at different electric fields at the MP2 level of theory for the ACCQ basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.069 663	−188.257 344	−188.346 989	−188.373 652	−188.360 718	−188.323 501	−188.271 547
0.001	−188.069 668	−188.257 350	−188.346 995	−188.373 658	−188.360 725	−188.323 508	−188.271 555
0.002	−188.069 683	−188.257 366	−188.347 012	−188.373 678	−188.360 746	−188.323 530	−188.271 578
0.003	−188.069 708	−188.257 394	−188.347 042	−188.373 710	−188.360 780	−188.323 568	−188.271 618
0.004	−188.069 744	−188.257 432	−188.347 084	−188.373 755	−188.360 829	−188.323 620	−188.271 674
0.005	−188.069 789	−188.257 482	−188.347 138	−188.373 813	−188.360 892	−188.323 687	−188.271 745
0.006	−188.069 845	−188.257 542	−188.347 204	−188.373 884	−188.360 968	−188.323 769	−188.271 833
0.007	−188.069 911	−188.257 614	−188.347 282	−188.373 969	−188.361 059	−188.323 866	−188.271 936
0.008	−188.069 987	−188.257 697	−188.347 371	−188.374 066	−188.361 163	−188.323 977	−188.272 055
0.009	−188.070 073	−188.257 791	−188.347 473	−188.374 175	−188.361 281	−188.324 104	−188.272 190
0.010	−188.070 169	−188.257 895	−188.347 587	−188.374 298	−188.361 413	−188.324 246	−188.272 341
0.015	−188.070 803	−188.258 585	−188.348 335	−188.375 107	−188.362 284	−188.325 178	−188.273 336
0.020	−188.071 692	−188.259 553	−188.349 385	−188.376 242	−188.363 505	−188.326 487	−188.274 732
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.069 663	−188.257 344	−188.346 989	−188.373 652	−188.360 718	−188.323 501	−188.271 547
0.001	−188.069 670	−188.257 352	−188.346 997	−188.373 662	−188.360 729	−188.323 513	−188.271 561
0.002	−188.069 691	−188.257 376	−188.347 024	−188.373 692	−188.360 763	−188.323 552	−188.271 604
0.003	−188.069 726	−188.257 415	−188.347 069	−188.373 742	−188.360 820	−188.323 616	−188.271 675
0.004	−188.069 776	−188.257 471	−188.347 131	−188.373 813	−188.360 899	−188.323 705	−188.271 776
0.005	−188.069 839	−188.257 542	−188.347 212	−188.373 904	−188.361 002	−188.323 820	−188.271 905
0.006	−188.069 917	−188.257 630	−188.347 310	−188.374 014	−188.361 127	−188.323 961	−188.272 062
0.007	−188.070 009	−188.257 733	−188.347 426	−188.374 145	−188.361 274	−188.324 127	−188.272 249
0.008	−188.070 115	−188.257 852	−188.347 560	−188.374 296	−188.361 445	−188.324 319	−188.272 463
0.009	−188.070 235	−188.257 986	−188.347 712	−188.374 468	−188.361 638	−188.324 537	−188.272 707
0.010	−188.070 369	−188.258 137	−188.347 882	−188.374 659	−188.361 854	−188.324 780	−188.272 979
0.015	−188.071 252	−188.259 130	−188.349 000	−188.375 919	−188.363 275	−188.326 381	−188.274 773
0.020	−188.072 491	−188.260 521	−188.350 567	−188.377 686	−188.365 268	−188.328 626	−188.277 287
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.069 663	−188.257 344	−188.346 989	−188.373 652	−188.360 718	−188.323 501	−188.271 547
0.001	−188.069 672	−188.257 354	−188.347 000	−188.373 666	−188.360 734	−188.323 519	−188.271 567
0.002	−188.069 699	−188.257 385	−188.347 036	−188.373 707	−188.360 781	−188.323 573	−188.271 629
0.003	−188.069 744	−188.257 437	−188.347 095	−188.373 775	−188.360 860	−188.323 664	−188.271 733
0.004	−188.069 808	−188.257 510	−188.347 179	−188.373 871	−188.360 970	−188.323 791	−188.271 878
0.005	−188.069 889	−188.257 603	−188.347 286	−188.373 994	−188.361 112	−188.323 954	−188.272 064
0.006	−188.069 989	−188.257 717	−188.347 416	−188.374 144	−188.361 285	−188.324 153	−188.272 292
0.007	−188.070 106	−188.257 851	−188.347 571	−188.374 322	−188.361 490	−188.324 389	−188.272 561
0.008	−188.070 242	−188.258 006	−188.347 749	−188.374 527	−188.361 726	−188.324 661	−188.272 872
0.009	−188.070 396	−188.258 182	−188.347 951	−188.374 760	−188.361 994	−188.324 969	−188.273 224
0.010	−188.070 568	−188.258 379	−188.348 177	−188.375 020	−188.362 294	−188.325 314	−188.273 618
0.015	−188.071 701	−188.259 674	−188.349 663	−188.376 730	−188.364 265	−188.327 582	−188.276 208
0.020	−188.073 288	−188.261 489	−188.351 746	−188.379 128	−188.367 028	−188.330 760	−188.279 837

Table A.14: The energies of CO_2 at different electric fields at the MP2 level of theory for the APC3 basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.070 435	−188.257 753	−188.347 103	−188.373 493	−188.360 282	−188.322 797	−188.270 600
0.001	−188.070 440	−188.257 758	−188.347 109	−188.373 500	−188.360 289	−188.322 805	−188.270 608
0.002	−188.070 455	−188.257 775	−188.347 127	−188.373 519	−188.360 310	−188.322 827	−188.270 632
0.003	−188.070 480	−188.257 802	−188.347 157	−188.373 551	−188.360 345	−188.322 864	−188.270 672
0.004	−188.070 516	−188.257 841	−188.347 199	−188.373 597	−188.360 394	−188.322 917	−188.270 728
0.005	−188.070 561	−188.257 891	−188.347 253	−188.373 655	−188.360 456	−188.322 984	−188.270 799
0.006	−188.070 617	−188.257 951	−188.347 318	−188.373 726	−188.360 533	−188.323 066	−188.270 887
0.007	−188.070 683	−188.258 023	−188.347 396	−188.373 810	−188.360 623	−188.323 163	−188.270 990
0.008	−188.070 759	−188.258 106	−188.347 486	−188.373 907	−188.360 728	−188.323 275	−188.271 110
0.009	−188.070 845	−188.258 199	−188.347 588	−188.374 017	−188.360 846	−188.323 402	−188.271 245
0.010	−188.070 941	−188.258 304	−188.347 701	−188.374 140	−188.360 979	−188.323 544	−188.271 397
0.015	−188.071 575	−188.258 994	−188.348 450	−188.374 950	−188.361 851	−188.324 478	−188.272 395
0.020	−188.072 464	−188.259 962	−188.349 500	−188.376 086	−188.363 074	−188.325 791	−188.273 796
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.070 435	−188.257 753	−188.347 103	−188.373 493	−188.360 282	−188.322 797	−188.270 600
0.001	−188.070 442	−188.257 761	−188.347 112	−188.373 503	−188.360 294	−188.322 810	−188.270 615
0.002	−188.070 463	−188.257 785	−188.347 139	−188.373 534	−188.360 328	−188.322 848	−188.270 658
0.003	−188.070 498	−188.257 824	−188.347 183	−188.373 584	−188.360 384	−188.322 912	−188.270 729
0.004	−188.070 548	−188.257 880	−188.347 246	−188.373 654	−188.360 464	−188.323 002	−188.270 829
0.005	−188.070 611	−188.257 951	−188.347 326	−188.373 745	−188.360 566	−188.323 117	−188.270 958
0.006	−188.070 689	−188.258 038	−188.347 425	−188.373 856	−188.360 691	−188.323 258	−188.271 116
0.007	−188.070 781	−188.258 141	−188.347 541	−188.373 987	−188.360 839	−188.323 424	−188.271 302
0.008	−188.070 886	−188.258 260	−188.347 675	−188.374 138	−188.361 009	−188.323 616	−188.271 518
0.009	−188.071 006	−188.258 395	−188.347 826	−188.374 309	−188.361 202	−188.323 834	−188.271 761
0.010	−188.071 141	−188.258 546	−188.347 996	−188.374 500	−188.361 418	−188.324 077	−188.272 034
0.015	−188.072 024	−188.259 538	−188.349 114	−188.375 761	−188.362 840	−188.325 679	−188.273 828
0.020	−188.073 263	−188.260 930	−188.350 681	−188.377 529	−188.364 835	−188.327 925	−188.276 345
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.070 435	−188.257 753	−188.347 103	−188.373 493	−188.360 282	−188.322 797	−188.270 600
0.001	−188.070 444	−188.257 763	−188.347 115	−188.373 507	−188.360 298	−188.322 815	−188.270 621
0.002	−188.070 471	−188.257 794	−188.347 151	−188.373 548	−188.360 345	−188.322 870	−188.270 683
0.003	−188.070 516	−188.257 846	−188.347 210	−188.373 616	−188.360 424	−188.322 960	−188.270 787
0.004	−188.070 580	−188.257 918	−188.347 293	−188.373 712	−188.360 534	−188.323 087	−188.270 931
0.005	−188.070 661	−188.258 011	−188.347 400	−188.373 835	−188.360 676	−188.323 250	−188.271 118
0.006	−188.070 761	−188.258 125	−188.347 531	−188.373 985	−188.360 849	−188.323 450	−188.271 345
0.007	−188.070 878	−188.258 260	−188.347 685	−188.374 163	−188.361 054	−188.323 685	−188.271 615
0.008	−188.071 014	−188.258 415	−188.347 863	−188.374 368	−188.361 290	−188.323 957	−188.271 925
0.009	−188.071 168	−188.258 591	−188.348 065	−188.374 601	−188.361 558	−188.324 266	−188.272 277
0.010	−188.071 340	−188.258 787	−188.348 291	−188.374 860	−188.361 858	−188.324 610	−188.272 671
0.015	−188.072 472	−188.260 082	−188.349 777	−188.376 571	−188.363 829	−188.326 878	−188.275 260
0.020	−188.074 060	−188.261 897	−188.351 860	−188.378 968	−188.366 591	−188.330 055	−188.278 889

Table A.15: The energies of CO_2 at different electric fields at the CCSD level of theory for the ACCT basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.011 539	−188.199 273	−188.287 280	−188.310 699	−188.293 393	−188.251 561	−188.196 188
0.001	−188.011 544	−188.199 278	−188.287 285	−188.310 705	−188.293 399	−188.251 568	−188.196 195
0.002	−188.011 558	−188.199 294	−188.287 303	−188.310 724	−188.293 420	−188.251 589	−188.196 218
0.003	−188.011 583	−188.199 321	−188.287 332	−188.310 755	−188.293 453	−188.251 625	−188.196 255
0.004	−188.011 618	−188.199 358	−188.287 372	−188.310 799	−188.293 500	−188.251 674	−188.196 308
0.005	−188.011 662	−188.199 407	−188.287 425	−188.310 855	−188.293 560	−188.251 738	−188.196 376
0.006	−188.011 716	−188.199 466	−188.287 488	−188.310 924	−188.293 633	−188.251 817	−188.196 459
0.007	−188.011 781	−188.199 535	−188.287 564	−188.311 005	−188.293 720	−188.251 909	−188.196 557
0.008	−188.011 855	−188.199 616	−188.287 651	−188.311 098	−188.293 821	−188.252 016	−188.196 670
0.009	−188.011 939	−188.199 707	−188.287 749	−188.311 205	−188.293 934	−188.252 137	−188.196 798
0.010	−188.012 033	−188.199 809	−188.287 860	−188.311 323	−188.294 061	−188.252 273	−188.196 941
0.015	−188.012 650	−188.200 480	−188.288 585	−188.312 105	−188.294 898	−188.253 164	−188.197 885
0.020	−188.013 516	−188.201 420	−188.289 603	−188.313 200	−188.296 071	−188.254 414	−188.199 209
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.011 539	−188.199 273	−188.287 280	−188.310 699	−188.293 393	−188.251 561	−188.196 188
0.001	−188.011 546	−188.199 280	−188.287 288	−188.310 709	−188.293 404	−188.251 572	−188.196 201
0.002	−188.011 566	−188.199 304	−188.287 314	−188.310 738	−188.293 436	−188.251 609	−188.196 241
0.003	−188.011 601	−188.199 342	−188.287 358	−188.310 786	−188.293 490	−188.251 669	−188.196 307
0.004	−188.011 650	−188.199 397	−188.287 419	−188.310 854	−188.293 566	−188.251 753	−188.196 400
0.005	−188.011 712	−188.199 466	−188.287 497	−188.310 942	−188.293 664	−188.251 861	−188.196 519
0.006	−188.011 788	−188.199 552	−188.287 592	−188.311 049	−188.293 783	−188.251 993	−188.196 665
0.007	−188.011 878	−188.199 653	−188.287 705	−188.311 175	−188.293 924	−188.252 150	−188.196 838
0.008	−188.011 982	−188.199 769	−188.287 836	−188.311 321	−188.294 086	−188.252 330	−188.197 037
0.009	−188.012 100	−188.199 901	−188.287 984	−188.311 486	−188.294 270	−188.252 534	−188.197 262
0.010	−188.012 231	−188.200 048	−188.288 149	−188.311 671	−188.294 476	−188.252 763	−188.197 514
0.015	−188.013 098	−188.201 019	−188.289 236	−188.312 887	−188.295 832	−188.254 267	−188.199 175
0.020	−188.014 313	−188.202 380	−188.290 760	−188.314 591	−188.297 732	−188.256 376	−188.201 502
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.011 539	−188.199 273	−188.287 280	−188.310 699	−188.293 393	−188.251 561	−188.196 188
0.001	−188.011 548	−188.199 283	−188.287 291	−188.310 712	−188.293 408	−188.251 577	−188.196 207
0.002	−188.011 574	−188.199 313	−188.287 326	−188.310 752	−188.293 453	−188.251 628	−188.196 264
0.003	−188.011 619	−188.199 364	−188.287 384	−188.310 818	−188.293 528	−188.251 713	−188.196 358
0.004	−188.011 681	−188.199 435	−188.287 465	−188.310 910	−188.293 632	−188.251 831	−188.196 491
0.005	−188.011 762	−188.199 526	−188.287 569	−188.311 029	−188.293 767	−188.251 984	−188.196 662
0.006	−188.011 860	−188.199 638	−188.287 696	−188.311 174	−188.293 932	−188.252 170	−188.196 871
0.007	−188.011 975	−188.199 770	−188.287 847	−188.311 345	−188.294 127	−188.252 390	−188.197 118
0.008	−188.012 109	−188.199 922	−188.288 021	−188.311 543	−188.294 352	−188.252 644	−188.197 403
0.009	−188.012 261	−188.200 095	−188.288 218	−188.311 768	−188.294 606	−188.252 931	−188.197 726
0.010	−188.012 430	−188.200 288	−188.288 438	−188.312 018	−188.294 891	−188.253 253	−188.198 087
0.015	−188.013 545	−188.201 558	−188.289 886	−188.313 668	−188.296 765	−188.255 370	−188.200 463
0.020	−188.015 108	−188.203 338	−188.291 916	−188.315 981	−188.299 390	−188.258 335	−188.203 792

Table A.16: The energies of CO_2 at different electric fields at the CCSD level of theory for the ACCQ basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.068 258	−188.252 137	−188.336 951	−188.357 864	−188.338 612	−188.295 270	−188.238 726
0.001	−188.068 263	−188.252 142	−188.336 957	−188.357 870	−188.338 618	−188.295 277	−188.238 733
0.002	−188.068 277	−188.252 159	−188.336 974	−188.357 889	−188.338 639	−188.295 299	−188.238 756
0.003	−188.068 302	−188.252 186	−188.337 003	−188.357 921	−188.338 672	−188.295 335	−188.238 794
0.004	−188.068 337	−188.252 223	−188.337 044	−188.357 965	−188.338 720	−188.295 385	−188.238 848
0.005	−188.068 382	−188.252 272	−188.337 097	−188.358 021	−188.338 780	−188.295 450	−188.238 916
0.006	−188.068 436	−188.252 331	−188.337 161	−188.358 091	−188.338 854	−188.295 529	−188.239 000
0.007	−188.068 501	−188.252 401	−188.337 237	−188.358 173	−188.338 942	−188.295 622	−188.239 099
0.008	−188.068 575	−188.252 482	−188.337 325	−188.358 267	−188.339 043	−188.295 730	−188.239 213
0.009	−188.068 660	−188.252 574	−188.337 424	−188.358 374	−188.339 158	−188.295 852	−188.239 343
0.010	−188.068 754	−188.252 677	−188.337 535	−188.358 494	−188.339 286	−188.295 989	−188.239 487
0.015	−188.069 376	−188.253 352	−188.338 266	−188.359 281	−188.340 130	−188.296 889	−188.240 441
0.020	−188.070 247	−188.254 299	−188.339 291	−188.360 386	−188.341 314	−188.298 151	−188.241 779
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.068 258	−188.252 137	−188.336 951	−188.357 864	−188.338 612	−188.295 270	−188.238 726
0.001	−188.068 264	−188.252 145	−188.336 960	−188.357 874	−188.338 623	−188.295 282	−188.238 739
0.002	−188.068 285	−188.252 168	−188.336 986	−188.357 903	−188.338 655	−188.295 318	−188.238 779
0.003	−188.068 320	−188.252 207	−188.337 029	−188.357 952	−188.338 709	−188.295 378	−188.238 845
0.004	−188.068 368	−188.252 261	−188.337 090	−188.358 020	−188.338 785	−188.295 463	−188.238 938
0.005	−188.068 431	−188.252 331	−188.337 168	−188.358 107	−188.338 883	−188.295 571	−188.239 058
0.006	−188.068 507	−188.252 416	−188.337 264	−188.358 214	−188.339 002	−188.295 703	−188.239 204
0.007	−188.068 597	−188.252 517	−188.337 377	−188.358 340	−188.339 143	−188.295 859	−188.239 376
0.008	−188.068 701	−188.252 634	−188.337 507	−188.358 486	−188.339 305	−188.296 040	−188.239 575
0.009	−188.068 819	−188.252 766	−188.337 655	−188.358 652	−188.339 489	−188.296 244	−188.239 801
0.010	−188.068 950	−188.252 913	−188.337 820	−188.358 836	−188.339 695	−188.296 473	−188.240 053
0.015	−188.069 817	−188.253 884	−188.338 908	−188.360 053	−188.341 051	−188.297 978	−188.241 715
0.020	−188.071 033	−188.255 245	−188.340 433	−188.361 758	−188.342 953	−188.300 088	−188.244 044
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.068 258	−188.252 137	−188.336 951	−188.357 864	−188.338 612	−188.295 270	−188.238 726
0.001	−188.068 266	−188.252 147	−188.336 962	−188.357 877	−188.338 627	−188.295 287	−188.238 745
0.002	−188.068 293	−188.252 178	−188.336 997	−188.357 917	−188.338 671	−188.295 338	−188.238 801
0.003	−188.068 338	−188.252 228	−188.337 055	−188.357 982	−188.338 746	−188.295 422	−188.238 896
0.004	−188.068 400	−188.252 299	−188.337 136	−188.358 074	−188.338 851	−188.295 540	−188.239 029
0.005	−188.068 480	−188.252 390	−188.337 239	−188.358 193	−188.338 985	−188.295 692	−188.239 199
0.006	−188.068 577	−188.252 501	−188.337 366	−188.358 337	−188.339 149	−188.295 877	−188.239 407
0.007	−188.068 693	−188.252 633	−188.337 516	−188.358 508	−188.339 343	−188.296 096	−188.239 653
0.008	−188.068 826	−188.252 785	−188.337 690	−188.358 706	−188.339 567	−188.296 349	−188.239 937
0.009	−188.068 977	−188.252 957	−188.337 886	−188.358 929	−188.339 821	−188.296 636	−188.240 259
0.010	−188.069 146	−188.253 149	−188.338 105	−188.359 179	−188.340 104	−188.296 957	−188.240 619
0.015	−188.070 258	−188.254 415	−188.339 549	−188.360 823	−188.341 972	−188.299 066	−188.242 987
0.020	−188.071 817	−188.256 190	−188.341 573	−188.363 128	−188.344 588	−188.302 021	−188.246 304

Table A.17: The energies of CO_2 at different electric fields at the CCSD level of theory for the APC3 basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.069 528	−188.253 079	−188.337 630	−188.358 294	−188.338 785	−188.295 196	−188.238 432
0.001	−188.069 533	−188.253 084	−188.337 635	−188.358 300	−188.338 791	−188.295 204	−188.238 440
0.002	−188.069 548	−188.253 101	−188.337 653	−188.358 319	−188.338 812	−188.295 225	−188.238 463
0.003	−188.069 573	−188.253 128	−188.337 682	−188.358 350	−188.338 845	−188.295 261	−188.238 501
0.004	−188.069 608	−188.253 165	−188.337 723	−188.358 394	−188.338 893	−188.295 311	−188.238 554
0.005	−188.069 652	−188.253 214	−188.337 776	−188.358 451	−188.338 953	−188.295 376	−188.238 623
0.006	−188.069 707	−188.253 273	−188.337 840	−188.358 520	−188.339 027	−188.295 455	−188.238 707
0.007	−188.069 771	−188.253 343	−188.337 916	−188.358 602	−188.339 115	−188.295 549	−188.238 806
0.008	−188.069 846	−188.253 424	−188.338 003	−188.358 696	−188.339 216	−188.295 657	−188.238 920
0.009	−188.069 930	−188.253 516	−188.338 103	−188.358 803	−188.339 331	−188.295 779	−188.239 050
0.010	−188.070 025	−188.253 619	−188.338 214	−188.358 923	−188.339 459	−188.295 916	−188.239 195
0.015	−188.070 646	−188.254 294	−188.338 945	−188.359 711	−188.340 304	−188.296 817	−188.240 150
0.020	−188.071 517	−188.255 240	−188.339 970	−188.360 816	−188.341 489	−188.298 081	−188.241 491
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.069 528	−188.253 079	−188.337 630	−188.358 294	−188.338 785	−188.295 196	−188.238 432
0.001	−188.069 535	−188.253 087	−188.337 638	−188.358 303	−188.338 795	−188.295 208	−188.238 445
0.002	−188.069 556	−188.253 110	−188.337 664	−188.358 332	−188.338 828	−188.295 244	−188.238 485
0.003	−188.069 591	−188.253 149	−188.337 708	−188.358 381	−188.338 882	−188.295 305	−188.238 552
0.004	−188.069 639	−188.253 203	−188.337 769	−188.358 449	−188.338 958	−188.295 389	−188.238 644
0.005	−188.069 701	−188.253 273	−188.337 847	−188.358 536	−188.339 055	−188.295 497	−188.238 764
0.006	−188.069 777	−188.253 358	−188.337 942	−188.358 643	−188.339 175	−188.295 629	−188.238 910
0.007	−188.069 867	−188.253 459	−188.338 055	−188.358 770	−188.339 315	−188.295 785	−188.239 082
0.008	−188.069 971	−188.253 575	−188.338 186	−188.358 915	−188.339 478	−188.295 966	−188.239 282
0.009	−188.070 089	−188.253 707	−188.338 333	−188.359 081	−188.339 662	−188.296 170	−188.239 507
0.010	−188.070 221	−188.253 855	−188.338 498	−188.359 265	−188.339 868	−188.296 399	−188.239 760
0.015	−188.071 087	−188.254 825	−188.339 586	−188.360 481	−188.341 224	−188.297 904	−188.241 422
0.020	−188.072 303	−188.256 186	−188.341 111	−188.362 187	−188.343 126	−188.300 015	−188.243 753
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.069 528	−188.253 079	−188.337 630	−188.358 294	−188.338 785	−188.295 196	−188.238 432
0.001	−188.069 537	−188.253 089	−188.337 641	−188.358 307	−188.338 800	−188.295 213	−188.238 451
0.002	−188.069 564	−188.253 120	−188.337 676	−188.358 346	−188.338 844	−188.295 264	−188.238 508
0.003	−188.069 608	−188.253 170	−188.337 733	−188.358 412	−188.338 919	−188.295 348	−188.238 602
0.004	−188.069 670	−188.253 241	−188.337 814	−188.358 504	−188.339 023	−188.295 466	−188.238 735
0.005	−188.069 750	−188.253 332	−188.337 918	−188.358 622	−188.339 157	−188.295 618	−188.238 905
0.006	−188.069 848	−188.253 443	−188.338 045	−188.358 766	−188.339 322	−188.295 803	−188.239 113
0.007	−188.069 963	−188.253 575	−188.338 195	−188.358 937	−188.339 515	−188.296 022	−188.239 359
0.008	−188.070 097	−188.253 726	−188.338 368	−188.359 134	−188.339 739	−188.296 275	−188.239 643
0.009	−188.070 248	−188.253 898	−188.338 564	−188.359 358	−188.339 993	−188.296 562	−188.239 965
0.010	−188.070 417	−188.254 091	−188.338 783	−188.359 608	−188.340 276	−188.296 882	−188.240 324
0.015	−188.071 528	−188.255 356	−188.340 226	−188.361 251	−188.342 143	−188.298 990	−188.242 691
0.020	−188.073 086	−188.257 131	−188.342 249	−188.363 555	−188.344 758	−188.301 945	−188.246 008

Table A.18: The energies of CO_2 at different electric fields at the CCSD(T) level of theory for the ACCT basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.031 502	−188.221 943	−188.313 187	−188.340 401	−188.327 429	−188.290 369	−188.239 995
0.001	−188.031 507	−188.221 949	−188.313 193	−188.340 407	−188.327 436	−188.290 376	−188.240 003
0.002	−188.031 522	−188.221 965	−188.313 211	−188.340 426	−188.327 456	−188.290 398	−188.240 026
0.003	−188.031 547	−188.221 992	−188.313 240	−188.340 458	−188.327 490	−188.290 434	−188.240 064
0.004	−188.031 582	−188.222 030	−188.313 281	−188.340 502	−188.327 538	−188.290 485	−188.240 118
0.005	−188.031 627	−188.222 079	−188.313 334	−188.340 559	−188.327 599	−188.290 550	−188.240 187
0.006	−188.031 682	−188.222 139	−188.313 399	−188.340 629	−188.327 674	−188.290 629	−188.240 271
0.007	−188.031 747	−188.222 210	−188.313 475	−188.340 712	−188.327 762	−188.290 723	−188.240 371
0.008	−188.031 822	−188.222 291	−188.313 564	−188.340 807	−188.327 864	−188.290 832	−188.240 486
0.009	−188.031 907	−188.222 383	−188.313 664	−188.340 914	−188.327 979	−188.290 955	−188.240 616
0.010	−188.032 002	−188.222 487	−188.313 775	−188.341 035	−188.328 108	−188.291 093	−188.240 762
0.015	−188.032 627	−188.223 166	−188.314 511	−188.341 828	−188.328 958	−188.291 999	−188.241 722
0.020	−188.033 504	−188.224 119	−188.315 543	−188.342 939	−188.330 150	−188.293 270	−188.243 070
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.031 502	−188.221 943	−188.313 187	−188.340 401	−188.327 429	−188.290 369	−188.239 995
0.001	−188.031 509	−188.221 951	−188.313 196	−188.340 411	−188.327 440	−188.290 381	−188.240 009
0.002	−188.031 530	−188.221 975	−188.313 222	−188.340 440	−188.327 473	−188.290 418	−188.240 049
0.003	−188.031 565	−188.222 014	−188.313 266	−188.340 490	−188.327 528	−188.290 479	−188.240 117
0.004	−188.031 614	−188.222 069	−188.313 328	−188.340 559	−188.327 605	−188.290 564	−188.240 212
0.005	−188.031 677	−188.222 140	−188.313 407	−188.340 647	−188.327 704	−188.290 674	−188.240 334
0.006	−188.031 754	−188.222 226	−188.313 504	−188.340 755	−188.327 825	−188.290 809	−188.240 483
0.007	−188.031 845	−188.222 328	−188.313 618	−188.340 883	−188.327 967	−188.290 968	−188.240 659
0.008	−188.031 950	−188.222 445	−188.313 750	−188.341 031	−188.328 132	−188.291 151	−188.240 862
0.009	−188.032 069	−188.222 579	−188.313 900	−188.341 198	−188.328 319	−188.291 359	−188.241 092
0.010	−188.032 202	−188.222 728	−188.314 067	−188.341 386	−188.328 528	−188.291 591	−188.241 349
0.015	−188.033 078	−188.223 710	−188.315 167	−188.342 617	−188.329 903	−188.293 120	−188.243 044
0.020	−188.034 306	−188.225 086	−188.316 710	−188.344 344	−188.331 831	−188.295 264	−188.245 420
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.031 502	−188.221 943	−188.313 187	−188.340 401	−188.327 429	−188.290 369	−188.239 995
0.001	−188.031 511	−188.221 954	−188.313 199	−188.340 414	−188.327 444	−188.290 386	−188.240 015
0.002	−188.031 538	−188.221 984	−188.313 234	−188.340 455	−188.327 490	−188.290 438	−188.240 073
0.003	−188.031 583	−188.222 036	−188.313 293	−188.340 521	−188.327 566	−188.290 524	−188.240 170
0.004	−188.031 646	−188.222 108	−188.313 374	−188.340 615	−188.327 672	−188.290 644	−188.240 306
0.005	−188.031 727	−188.222 200	−188.313 480	−188.340 735	−188.327 809	−188.290 799	−188.240 480
0.006	−188.031 826	−188.222 313	−188.313 609	−188.340 882	−188.327 976	−188.290 988	−188.240 694
0.007	−188.031 943	−188.222 446	−188.313 761	−188.341 055	−188.328 173	−188.291 212	−188.240 946
0.008	−188.032 078	−188.222 600	−188.313 936	−188.341 256	−188.328 401	−188.291 470	−188.241 238
0.009	−188.032 231	−188.222 774	−188.314 135	−188.341 483	−188.328 659	−188.291 762	−188.241 568
0.010	−188.032 402	−188.222 969	−188.314 358	−188.341 736	−188.328 948	−188.292 089	−188.241 937
0.015	−188.033 528	−188.224 252	−188.315 822	−188.343 406	−188.330 847	−188.294 241	−188.244 364
0.020	−188.035 107	−188.226 051	−188.317 875	−188.345 747	−188.333 508	−188.297 256	−188.247 766

Table A.19: The energies of CO_2 at different electric fields at the CCSD(T) level of theory for the ACCQ basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.090 091	−188.276 707	−188.364 797	−188.389 557	−188.374 698	−188.336 194	−188.284 717
0.001	−188.090 096	−188.276 713	−188.364 803	−188.389 563	−188.374 705	−188.336 201	−188.284 725
0.002	−188.090 111	−188.276 729	−188.364 821	−188.389 582	−188.374 726	−188.336 223	−188.284 748
0.003	−188.090 136	−188.276 756	−188.364 851	−188.389 614	−188.374 760	−188.336 260	−188.284 787
0.004	−188.090 171	−188.276 795	−188.364 892	−188.389 659	−188.374 808	−188.336 311	−188.284 841
0.005	−188.090 217	−188.276 844	−188.364 945	−188.389 716	−188.374 870	−188.336 377	−188.284 911
0.006	−188.090 272	−188.276 904	−188.365 011	−188.389 787	−188.374 945	−188.336 457	−188.284 996
0.007	−188.090 337	−188.276 975	−188.365 088	−188.389 870	−188.375 034	−188.336 552	−188.285 097
0.008	−188.090 413	−188.277 057	−188.365 177	−188.389 966	−188.375 137	−188.336 662	−188.285 213
0.009	−188.090 498	−188.277 150	−188.365 277	−188.390 074	−188.375 253	−188.336 786	−188.285 345
0.010	−188.090 594	−188.277 254	−188.365 390	−188.390 196	−188.375 384	−188.336 925	−188.285 492
0.015	−188.091 224	−188.277 939	−188.366 132	−188.390 996	−188.376 242	−188.337 840	−188.286 463
0.020	−188.092 106	−188.278 899	−188.367 172	−188.392 117	−188.377 445	−188.339 124	−188.287 825
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.090 091	−188.276 707	−188.364 797	−188.389 557	−188.374 698	−188.336 194	−188.284 717
0.001	−188.090 098	−188.276 715	−188.364 806	−188.389 566	−188.374 709	−188.336 206	−188.284 730
0.002	−188.090 119	−188.276 738	−188.364 833	−188.389 596	−188.374 742	−188.336 243	−188.284 771
0.003	−188.090 154	−188.276 778	−188.364 876	−188.389 645	−188.374 797	−188.336 304	−188.284 839
0.004	−188.090 203	−188.276 833	−188.364 938	−188.389 714	−188.374 874	−188.336 390	−188.284 934
0.005	−188.090 266	−188.276 903	−188.365 017	−188.389 803	−188.374 973	−188.336 500	−188.285 056
0.006	−188.090 343	−188.276 990	−188.365 114	−188.389 911	−188.375 094	−188.336 634	−188.285 205
0.007	−188.090 434	−188.277 092	−188.365 229	−188.390 039	−188.375 237	−188.336 793	−188.285 381
0.008	−188.090 539	−188.277 210	−188.365 361	−188.390 187	−188.375 402	−188.336 977	−188.285 585
0.009	−188.090 658	−188.277 343	−188.365 510	−188.390 355	−188.375 589	−188.337 185	−188.285 815
0.010	−188.090 791	−188.277 492	−188.365 678	−188.390 542	−188.375 798	−188.337 417	−188.286 073
0.015	−188.091 668	−188.278 475	−188.366 779	−188.391 775	−188.377 175	−188.338 948	−188.287 770
0.020	−188.092 898	−188.279 852	−188.368 323	−188.393 504	−188.379 105	−188.341 095	−188.290 149
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.090 091	−188.276 707	−188.364 797	−188.389 557	−188.374 698	−188.336 194	−188.284 717
0.001	−188.090 100	−188.276 717	−188.364 809	−188.389 570	−188.374 713	−188.336 211	−188.284 736
0.002	−188.090 127	−188.276 748	−188.364 844	−188.389 610	−188.374 759	−188.336 262	−188.284 794
0.003	−188.090 172	−188.276 799	−188.364 902	−188.389 676	−188.374 834	−188.336 348	−188.284 891
0.004	−188.090 234	−188.276 871	−188.364 984	−188.389 770	−188.374 940	−188.336 468	−188.285 027
0.005	−188.090 315	−188.276 963	−188.365 089	−188.389 889	−188.375 077	−188.336 623	−188.285 201
0.006	−188.090 414	−188.277 075	−188.365 218	−188.390 036	−188.375 243	−188.336 811	−188.285 414
0.007	−188.090 531	−188.277 208	−188.365 369	−188.390 209	−188.375 440	−188.337 034	−188.285 666
0.008	−188.090 665	−188.277 362	−188.365 544	−188.390 409	−188.375 667	−188.337 292	−188.285 956
0.009	−188.090 818	−188.277 536	−188.365 743	−188.390 635	−188.375 925	−188.337 583	−188.286 285
0.010	−188.090 989	−188.277 730	−188.365 965	−188.390 888	−188.376 212	−188.337 909	−188.286 653
0.015	−188.092 112	−188.279 010	−188.367 426	−188.392 553	−188.378 106	−188.340 055	−188.289 075
0.020	−188.093 688	−188.280 805	−188.369 473	−188.394 887	−188.380 761	−188.343 062	−188.292 468

Table A.20: The energies of CO_2 at different electric fields at the CCSD(T) level of theory for the APC3 basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.091 296	−188.277 567	−188.365 378	−188.389 874	−188.374 747	−188.335 983	−188.284 275
0.001	−188.091 301	−188.277 572	−188.365 384	−188.389 881	−188.374 753	−188.335 990	−188.284 283
0.002	−188.091 316	−188.277 589	−188.365 402	−188.389 900	−188.374 774	−188.336 012	−188.284 306
0.003	−188.091 341	−188.277 616	−188.365 431	−188.389 932	−188.374 808	−188.336 049	−188.284 345
0.004	−188.091 376	−188.277 654	−188.365 473	−188.389 977	−188.374 856	−188.336 100	−188.284 399
0.005	−188.091 421	−188.277 703	−188.365 526	−188.390 034	−188.374 918	−188.336 166	−188.284 469
0.006	−188.091 477	−188.277 764	−188.365 591	−188.390 104	−188.374 993	−188.336 246	−188.284 554
0.007	−188.091 542	−188.277 835	−188.365 668	−188.390 187	−188.375 082	−188.336 341	−188.284 655
0.008	−188.091 617	−188.277 917	−188.365 757	−188.390 283	−188.375 185	−188.336 451	−188.284 772
0.009	−188.091 703	−188.278 010	−188.365 858	−188.390 392	−188.375 302	−188.336 576	−188.284 904
0.010	−188.091 799	−188.278 114	−188.365 970	−188.390 513	−188.375 432	−188.336 715	−188.285 051
0.015	−188.092 428	−188.278 798	−188.366 712	−188.391 313	−188.376 291	−188.337 631	−188.286 024
0.020	−188.093 310	−188.279 758	−188.367 752	−188.392 436	−188.377 496	−188.338 917	−188.287 389
XZ-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.091 296	−188.277 567	−188.365 378	−188.389 874	−188.374 747	−188.335 983	−188.284 275
0.001	−188.091 303	−188.277 575	−188.365 387	−188.389 884	−188.374 758	−188.335 995	−188.284 288
0.002	−188.091 324	−188.277 598	−188.365 413	−188.389 914	−188.374 791	−188.336 032	−188.284 329
0.003	−188.091 359	−188.277 637	−188.365 457	−188.389 963	−188.374 846	−188.336 093	−188.284 397
0.004	−188.091 408	−188.277 692	−188.365 519	−188.390 032	−188.374 922	−188.336 179	−188.284 492
0.005	−188.091 471	−188.277 763	−188.365 598	−188.390 121	−188.375 021	−188.336 289	−188.284 614
0.006	−188.091 548	−188.277 849	−188.365 695	−188.390 229	−188.375 142	−188.336 423	−188.284 763
0.007	−188.091 639	−188.277 951	−188.365 809	−188.390 357	−188.375 285	−188.336 582	−188.284 939
0.008	−188.091 744	−188.278 069	−188.365 941	−188.390 505	−188.375 450	−188.336 766	−188.285 143
0.009	−188.091 863	−188.278 202	−188.366 091	−188.390 672	−188.375 637	−188.336 974	−188.285 373
0.010	−188.091 996	−188.278 352	−188.366 258	−188.390 859	−188.375 846	−188.337 206	−188.285 631
0.015	−188.092 872	−188.279 334	−188.367 359	−188.392 092	−188.377 223	−188.338 738	−188.287 328
0.020	−188.094 102	−188.280 711	−188.368 903	−188.393 821	−188.379 153	−188.340 886	−188.289 710
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	−188.091 296	−188.277 567	−188.365 378	−188.389 874	−188.374 747	−188.335 983	−188.284 275
0.001	−188.091 305	−188.277 577	−188.365 390	−188.389 888	−188.374 762	−188.336 000	−188.284 294
0.002	−188.091 332	−188.277 608	−188.365 425	−188.389 928	−188.374 807	−188.336 052	−188.284 352
0.003	−188.091 376	−188.277 659	−188.365 483	−188.389 994	−188.374 883	−188.336 137	−188.284 449
0.004	−188.091 439	−188.277 730	−188.365 565	−188.390 087	−188.374 989	−188.336 257	−188.284 584
0.005	−188.091 520	−188.277 822	−188.365 670	−188.390 207	−188.375 125	−188.336 412	−188.284 759
0.006	−188.091 619	−188.277 935	−188.365 798	−188.390 353	−188.375 291	−188.336 600	−188.284 971
0.007	−188.091 735	−188.278 068	−188.365 950	−188.390 526	−188.375 488	−188.336 823	−188.285 223
0.008	−188.091 870	−188.278 221	−188.366 125	−188.390 726	−188.375 715	−188.337 080	−188.285 513
0.009	−188.092 023	−188.278 395	−188.366 323	−188.390 952	−188.375 972	−188.337 372	−188.285 842
0.010	−188.092 193	−188.278 589	−188.366 545	−188.391 205	−188.376 260	−188.337 698	−188.286 210
0.015	−188.093 317	−188.279 869	−188.368 005	−188.392 870	−188.378 153	−188.339 843	−188.288 631
0.020	−188.094 891	−188.281 663	−188.370 052	−188.395 203	−188.380 806	−188.342 849	−188.292 023

A.5 Dipole Moments of CO_2 Used to Calculate Polarizabilities and Hyperpolarizabilities

Table A.21: The x-direction and z-direction dipole moments of CO_2 at different electric fields at the RHF level of theory for the ACCT basis set.

			X-Direction				
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.009 341	0.010 148	0.010 974	0.011 807	0.012 634	0.013 441	0.014 213
0.002	0.018 682	0.020 295	0.021 949	0.023 615	0.025 27	0.026 883	0.028 426
0.003	0.028 024	0.030 444	0.032 924	0.035 424	0.037 906	0.040 327	0.042 641
0.004	0.037 366	0.040 594	0.043 901	0.047 235	0.050 544	0.053 773	0.056 859
0.005	0.046 71	0.050 745	0.054 879	0.059 048	0.063 185	0.067 221	0.071 08
0.006	0.056 055	0.060 898	0.065 86	0.070 863	0.075 829	0.080 674	0.085 305
0.007	0.065 403	0.071 054	0.076 844	0.082 682	0.088 477	0.094 131	0.099 535
0.008	0.074 752	0.081 212	0.087 83	0.094 504	0.101 129	0.107 592	0.113 771
0.009	0.084 104	0.091 373	0.098 821	0.106 331	0.113 786	0.121 06	0.128 014
0.010	0.093 459	0.101 537	0.109 815	0.118 162	0.126 449	0.134 535	0.142 264
			Z-Direction				
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.016 481	0.018 623	0.021 023	0.023 656	0.026 485	0.029 472	0.032 592
0.002	0.032 963	0.037 246	0.042 048	0.047 312	0.052 969	0.058 942	0.065 185
0.003	0.049 445	0.055 871	0.063 072	0.070 969	0.079 455	0.088 415	0.097 78
0.004	0.065 929	0.074 497	0.084 099	0.094 628	0.105 944	0.117 89	0.130 379
0.005	0.082 416	0.093 125	0.105 128	0.118 291	0.132 435	0.147 369	0.162 982
0.006	0.098 905	0.111 756	0.126 161	0.141 957	0.158 931	0.176 852	0.195 589
0.007	0.115 398	0.130 392	0.147 196	0.165 627	0.185 431	0.206 34	0.228 201
0.008	0.131 895	0.149 031	0.168 238	0.189 302	0.211 936	0.235 833	0.260 82
0.009	0.148 397	0.167 676	0.189 286	0.212 982	0.238 447	0.265 334	0.293 447
0.010	0.164 904	0.186 326	0.210 338	0.236 669	0.264 965	0.294 841	0.326 083

Table A.22: The xz-direction (x-component and z-component) dipole moments of CO_2 at different electric fields at the RHF level of theory for the ACCT basis set.

XZ-Direction (X Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.006 605	0.007 175	0.007 76	0.008 349	0.008 934	0.009 505	0.010 05
0.002	0.013 21	0.014 351	0.015 52	0.016 699	0.017 868	0.019 01	0.0201
0.003	0.019 816	0.021 527	0.023 281	0.025 049	0.026 804	0.028 516	0.030 153
0.004	0.026 423	0.028 705	0.031 043	0.033 401	0.035 741	0.038 024	0.040 207
0.005	0.033 03	0.035 884	0.038 807	0.041 755	0.044 681	0.047 535	0.050 264
0.006	0.039 64	0.043 064	0.046 573	0.050 111	0.053 623	0.057 049	0.060 325
0.007	0.046 251	0.050 247	0.054 341	0.058 47	0.062 568	0.066 567	0.070 39
0.008	0.052 865	0.057 432	0.062 112	0.066 832	0.071 517	0.076 09	0.080 461
0.009	0.059 48	0.064 62	0.069 887	0.075 198	0.080 471	0.085 617	0.090 538
0.010	0.066 099	0.071 811	0.077 665	0.083 568	0.089 43	0.095 151	0.100 622
XZ-Direction (Z Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.011 654	0.013 169	0.014 866	0.016 727	0.018 728	0.020 84	0.023 046
0.002	0.023 308	0.026 337	0.029 732	0.033 455	0.037 455	0.041 679	0.046 093
0.003	0.034 963	0.039 507	0.0446	0.050 183	0.056 184	0.062 519	0.069 141
0.004	0.046 619	0.052 677	0.059 467	0.066 913	0.074 914	0.083 362	0.092 192
0.005	0.058 277	0.065 85	0.074 337	0.083 645	0.093 647	0.104 207	0.115 247
0.006	0.069 936	0.079 024	0.089 21	0.100 379	0.112 383	0.125 056	0.138 306
0.007	0.081 598	0.092 201	0.104 085	0.117 117	0.131 122	0.145 909	0.161 369
0.008	0.093 263	0.105 381	0.118 964	0.133 859	0.149 866	0.166 767	0.184 438
0.009	0.104 931	0.118 564	0.133 845	0.150 605	0.168 614	0.187 63	0.207 513
0.010	0.116 602	0.131 752	0.148 732	0.167 355	0.187 368	0.208 499	0.230 595

Table A.23: The x-direction and z-direction dipole moments of CO_2 at different electric fields at the RHF level of theory for the ACCQ basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.009 424	0.010 245	0.011 088	0.011 939	0.012 784	0.013 609	0.014 399
0.002	0.018 848	0.020 491	0.022 177	0.023 878	0.025 568	0.027 218	0.028 798
0.003	0.028 273	0.030 737	0.033 266	0.035 819	0.038 354	0.040 83	0.0432
0.004	0.0377	0.040 985	0.044 357	0.047 762	0.051 143	0.054 444	0.057 604
0.005	0.047 127	0.051 235	0.055 451	0.059 707	0.063 934	0.068 061	0.072 013
0.006	0.056 557	0.061 486	0.066 547	0.071 655	0.076 729	0.081 683	0.086 426
0.007	0.065 989	0.071 741	0.077 646	0.083 607	0.089 528	0.095 31	0.100 846
0.008	0.075 423	0.081 999	0.088 749	0.095 564	0.102 333	0.108 943	0.115 272
0.009	0.084 861	0.092 26	0.099 857	0.107 526	0.115 144	0.122 583	0.129 707
0.010	0.094 302	0.102 525	0.110 969	0.119 493	0.127 962	0.136 231	0.144 15
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.016 486	0.018 626	0.021 023	0.023 651	0.026 479	0.029 469	0.032 596
0.002	0.032 972	0.037 252	0.042 046	0.047 303	0.052 958	0.058 937	0.065 194
0.003	0.049 459	0.055 88	0.063 07	0.070 956	0.079 439	0.088 407	0.097 794
0.004	0.065 949	0.074 51	0.084 096	0.094 612	0.105 922	0.117 88	0.130 398
0.005	0.082 441	0.093 142	0.105 125	0.118 27	0.132 409	0.147 357	0.163 006
0.006	0.098 936	0.111 778	0.126 158	0.141 933	0.158 901	0.176 839	0.195 619
0.007	0.115 435	0.130 418	0.147 197	0.165 601	0.185 398	0.206 327	0.228 239
0.008	0.131 939	0.149 063	0.168 24	0.189 274	0.2119	0.235 821	0.260 866
0.009	0.148 449	0.167 713	0.189 289	0.212 954	0.238 41	0.265 323	0.293 503
0.010	0.164 964	0.186 37	0.210 345	0.236 641	0.264 927	0.294 834	0.326 149

Table A.24: The xz-direction (x-component and z-component) dipole moments of CO_2 at different electric fields at the RHF level of theory for the ACCQ basis set.

XZ-Direction (X Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.006 664	0.007 244	0.007 84	0.008 442	0.009 04	0.009 623	0.010 181
0.002	0.013 328	0.014 489	0.015 681	0.016 885	0.018 08	0.019 247	0.020 364
0.003	0.019 993	0.021 735	0.023 523	0.025 328	0.027 121	0.028 872	0.030 548
0.004	0.026 658	0.028 982	0.031 367	0.033 774	0.036 165	0.038 499	0.040 734
0.005	0.033 326	0.036 23	0.039 212	0.042 221	0.045 21	0.048 129	0.050 924
0.006	0.039 995	0.043 481	0.047 059	0.050 672	0.054 26	0.057 764	0.061 119
0.007	0.046 666	0.050 734	0.054 91	0.059 125	0.063 313	0.067 402	0.071 318
0.008	0.053 34	0.057 99	0.062 763	0.067 583	0.072 37	0.077 046	0.081 524
0.009	0.060 017	0.065 249	0.070 621	0.076 045	0.081 433	0.086 696	0.091 737
0.010	0.066 697	0.072 512	0.078 483	0.084 512	0.090 502	0.096 353	0.101 957
XZ-Direction (Z Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0	0	0	0	0	0	0
0.001	0.011 657	0.013 17	0.014 865	0.016 724	0.018 724	0.020 838	0.023 049
0.002	0.023 315	0.026 342	0.029 731	0.033 449	0.037 447	0.041 675	0.046 099
0.003	0.034 973	0.039 513	0.044 599	0.050 174	0.056 172	0.062 514	0.069 151
0.004	0.046 633	0.052 687	0.059 466	0.066 901	0.074 899	0.083 355	0.092 206
0.005	0.058 295	0.065 862	0.074 335	0.083 631	0.093 629	0.104 199	0.115 265
0.006	0.069 958	0.079 04	0.089 208	0.100 364	0.112 362	0.125 048	0.138 328
0.007	0.081 625	0.092 22	0.104 084	0.1171	0.1311	0.145 901	0.161 397
0.008	0.093 295	0.105 404	0.118 965	0.133 841	0.149 842	0.166 76	0.184 472
0.009	0.104 968	0.118 592	0.133 849	0.150 587	0.168 59	0.187 625	0.207 554
0.010	0.116 646	0.131 785	0.148 74	0.167 338	0.187 344	0.208 497	0.230 645

Table A.25: The x-direction and z-direction dipole moments of CO_2 at different electric fields at the RHF level of theory for the APC3 basis set.

			X-Direction				
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.009 434	0.010 256	0.011 100	0.011 954	0.012 802	0.013 631	0.014 426
0.002	0.018 869	0.020 512	0.022 201	0.023 908	0.025 605	0.027 263	0.028 852
0.003	0.028 304	0.030 770	0.033 304	0.035 864	0.038 410	0.040 897	0.043 281
0.004	0.037 741	0.041 029	0.044 408	0.047 823	0.051 217	0.054 534	0.057 714
0.005	0.047 179	0.051 290	0.055 515	0.059 784	0.064 028	0.068 176	0.072 152
0.006	0.056 620	0.061 554	0.066 625	0.071 749	0.076 843	0.081 823	0.086 595
0.007	0.066 063	0.071 821	0.077 739	0.083 719	0.089 664	0.095 476	0.101 046
0.008	0.075 510	0.082 091	0.088 857	0.095 694	0.102 491	0.109 136	0.115 505
0.009	0.084 960	0.092 366	0.099 980	0.107 675	0.115 326	0.122 805	0.129 974
0.010	0.094 414	0.102 646	0.111 109	0.119 663	0.128 168	0.136 483	0.144 454
			Z-Direction				
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.016 485	0.018 624	0.021 019	0.023 646	0.026 470	0.029 457	0.032 585
0.002	0.032 971	0.037 248	0.042 038	0.047 292	0.052 942	0.058 916	0.065 170
0.003	0.049 458	0.055 874	0.063 059	0.070 939	0.079 415	0.088 376	0.097 759
0.004	0.065 947	0.074 502	0.084 082	0.094 590	0.105 891	0.117 840	0.130 352
0.005	0.082 439	0.093 134	0.105 109	0.118 244	0.132 371	0.147 308	0.162 950
0.006	0.098 934	0.111 769	0.126 14	0.141 902	0.158 856	0.176 781	0.195 553
0.007	0.115 435	0.130 408	0.147 175	0.165 566	0.185 346	0.206 26	0.228 164
0.008	0.131 94	0.149 053	0.168 217	0.189 236	0.211 843	0.235 747	0.260 783
0.009	0.148 451	0.167 704	0.189 265	0.212 913	0.238 348	0.265 243	0.293 412
0.010	0.164 968	0.186 362	0.210 32	0.236 598	0.264 862	0.294 749	0.326 052

Table A.26: The xz-direction (x-component and z-component) dipole moments of CO_2 at different electric fields at the RHF level of theory for the APC3 basis set.

XZ-Direction (X Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.006 671	0.007 252	0.007 849	0.008 453	0.009 052	0.009 639	0.010 200
0.002	0.013 342	0.014 504	0.015 699	0.016 906	0.018 106	0.019 278	0.020 402
0.003	0.020 014	0.021 758	0.023 550	0.025 360	0.027 160	0.028 919	0.030 605
0.004	0.026 688	0.029 013	0.031 402	0.033 817	0.036 217	0.038 563	0.040 812
0.005	0.033 363	0.036 270	0.039 257	0.042 276	0.045 277	0.048 211	0.051 023
0.006	0.040 040	0.043 529	0.047 115	0.050 738	0.054 341	0.057 863	0.061 238
0.007	0.046 720	0.050 791	0.054 976	0.059 205	0.063 409	0.067 520	0.071 460
0.008	0.053 402	0.058 056	0.062 840	0.067 675	0.072 483	0.077 183	0.081 690
0.009	0.060 089	0.065 326	0.070 710	0.076 151	0.081 563	0.086 854	0.091 927
0.010	0.066 779	0.072 600	0.078 584	0.084 634	0.090 650	0.096 532	0.102 174
XZ-Direction (Z Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.011 657	0.013 169	0.014 863	0.016 720	0.018 718	0.020 830	0.023 041
0.002	0.023 314	0.026 339	0.029 726	0.033 441	0.037 436	0.041 660	0.046 083
0.003	0.034 972	0.039 509	0.044 591	0.050 162	0.056 156	0.062 492	0.069 127
0.004	0.046 632	0.052 681	0.059 456	0.066 886	0.074 877	0.083 327	0.092 174
0.005	0.058 293	0.065 856	0.074 324	0.083 613	0.093 602	0.104 165	0.115 226
0.006	0.069 958	0.079 033	0.089 196	0.100 343	0.112 331	0.125 008	0.138 283
0.007	0.081 625	0.092 214	0.104 071	0.117 077	0.131 065	0.145 856	0.161 346
0.008	0.093 296	0.105 399	0.118 951	0.133 816	0.149 805	0.166 711	0.184 416
0.009	0.104 972	0.118 588	0.133 836	0.150 561	0.168 550	0.187 572	0.207 495
0.010	0.116 652	0.131 782	0.148 726	0.167 312	0.187 303	0.208 442	0.230 583

Table A.27: The x-direction and z-direction dipole moments of CO_2 at different electric fields at the MP2 level of theory for the ACCT basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.010 044	0.010 924	0.011 842	0.012 786	0.013 745	0.014 708	0.015 668
0.002	0.020 089	0.021 849	0.023 685	0.025 573	0.027 491	0.029 418	0.031 337
0.003	0.030 134	0.032 775	0.035 529	0.038 362	0.041 239	0.044 128	0.047 009
0.004	0.040 181	0.043 703	0.047 375	0.051 152	0.054 989	0.058 843	0.062 684
0.005	0.050 230	0.054 633	0.059 224	0.063 946	0.068 743	0.073 562	0.078 364
0.006	0.060 280	0.065 564	0.071 075	0.076 743	0.082 501	0.088 286	0.094 051
0.007	0.070 333	0.076 499	0.082 930	0.089 545	0.096 265	0.103 016	0.109 745
0.008	0.080 389	0.087 438	0.094 789	0.102 352	0.110 034	0.117 754	0.125 448
0.009	0.090 448	0.098 380	0.106 653	0.115 164	0.123 811	0.132 499	0.141 160
0.010	0.100 511	0.109 327	0.118 523	0.127 983	0.137 596	0.147 255	0.156 884
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.018 111	0.020 707	0.023 778	0.027 377	0.031 552	0.036 301	0.041 449
0.002	0.036 224	0.041 414	0.047 556	0.054 755	0.063 104	0.072 602	0.082 900
0.003	0.054 337	0.062 124	0.071 336	0.082 133	0.094 659	0.108 906	0.124 353
0.004	0.072 454	0.082 836	0.095 120	0.109 516	0.126 216	0.145 212	0.165 812
0.005	0.090 574	0.103 551	0.118 906	0.136 902	0.157 777	0.181 522	0.207 273
0.006	0.108 698	0.124 272	0.142 698	0.164 293	0.189 344	0.217 837	0.248 738
0.007	0.126 827	0.144 997	0.166 495	0.191 689	0.220 915	0.254 158	0.290 208
0.008	0.144 962	0.165 728	0.190 299	0.219 093	0.252 494	0.290 485	0.331 686
0.009	0.163 103	0.186 467	0.214 110	0.246 504	0.284 080	0.326 820	0.373 171
0.010	0.181 253	0.207 214	0.237 930	0.273 924	0.315 676	0.363 164	0.414 665

Table A.28: The xz-direction (x-component and z-component) dipole moments of CO_2 at different electric fields at the MP2 level of theory for the ACCT basis set.

XZ-Direction (X Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.007 042	0.007 659	0.008 302	0.008 964	0.009 636	0.010 311	0.010 984
0.002	0.014 205	0.015 450	0.016 748	0.018 083	0.019 439	0.020 801	0.022 159
0.003	0.021 309	0.023 176	0.025 124	0.027 126	0.029 161	0.031 204	0.033 241
0.004	0.028 414	0.030 904	0.033 501	0.036 172	0.038 884	0.041 610	0.044 326
0.005	0.035 520	0.038 633	0.041 880	0.045 220	0.048 611	0.052 019	0.055 414
0.006	0.042 629	0.046 366	0.050 262	0.054 271	0.058 342	0.062 432	0.066 508
0.007	0.049 740	0.054 101	0.058 648	0.063 326	0.068 078	0.072 852	0.077 608
0.008	0.056 855	0.061 839	0.067 037	0.072 385	0.077 819	0.083 277	0.088 715
0.009	0.063 972	0.069 581	0.075 432	0.081 451	0.087 565	0.093 709	0.099 830
0.010	0.071 094	0.077 327	0.083 831	0.090 521	0.097 319	0.104 149	0.110 955
XZ-Direction (Z Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.012 807	0.014 642	0.016 813	0.019 358	0.022 311	0.025 669	0.029 309
0.002	0.025 614	0.029 285	0.033 627	0.038 717	0.044 621	0.051 338	0.058 619
0.003	0.038 423	0.043 928	0.050 443	0.058 078	0.066 934	0.077 009	0.087 931
0.004	0.051 233	0.058 574	0.067 260	0.077 440	0.089 250	0.102 683	0.117 246
0.005	0.064 045	0.073 222	0.084 080	0.096 806	0.111 568	0.128 360	0.146 567
0.006	0.076 860	0.087 873	0.100 903	0.116 175	0.133 890	0.154 041	0.175 892
0.007	0.089 679	0.102 528	0.117 731	0.135 548	0.156 217	0.179 727	0.205 221
0.008	0.102 502	0.117 187	0.134 563	0.154 927	0.178 550	0.205 420	0.234 557
0.009	0.115 329	0.131 851	0.151 401	0.174 312	0.200 890	0.231 119	0.263 900
0.010	0.128 161	0.146 521	0.168 245	0.193 704	0.223 236	0.256 826	0.293 251

Table A.29: The x-direction and z-direction dipole moments of CO_2 at different electric fields at the MP2 level of theory for the ACCQ basis set.

X-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.010 128	0.011 023	0.011 959	0.012 923	0.013 904	0.014 892	0.015 880
0.002	0.020 257	0.022 047	0.023 919	0.025 847	0.027 809	0.029 785	0.031 761
0.003	0.030 386	0.033 072	0.035 880	0.038 773	0.041 717	0.044 681	0.047 645
0.004	0.040 517	0.044 099	0.047 843	0.051 701	0.055 627	0.059 581	0.063 534
0.005	0.050 650	0.055 128	0.059 809	0.064 633	0.069 542	0.074 485	0.079 428
0.006	0.060 786	0.066 160	0.071 779	0.077 569	0.083 461	0.089 396	0.095 330
0.007	0.070 925	0.077 196	0.083 752	0.090 510	0.097 388	0.104 314	0.111 241
0.008	0.081 067	0.088 236	0.095 731	0.103 457	0.111 321	0.119 241	0.127 161
0.009	0.091 213	0.099 280	0.107 716	0.116 412	0.125 263	0.134 178	0.143 094
0.010	0.101 364	0.110 330	0.119 707	0.129 374	0.139 214	0.149 126	0.159 040
Z-Direction							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.018 098	0.020 691	0.023 756	0.027 347	0.031 515	0.036 261	0.041 411
0.002	0.036 197	0.041 383	0.047 513	0.054 695	0.063 032	0.072 524	0.082 823
0.003	0.054 298	0.062 077	0.071 271	0.082 045	0.094 551	0.108 789	0.124 238
0.004	0.072 401	0.082 774	0.095 033	0.109 398	0.126 073	0.145 057	0.165 660
0.005	0.090 508	0.103 475	0.118 799	0.136 756	0.157 600	0.181 330	0.207 085
0.006	0.108 620	0.124 181	0.142 570	0.164 120	0.189 132	0.217 608	0.248 515
0.007	0.126 738	0.144 893	0.166 348	0.191 490	0.220 671	0.253 894	0.289 953
0.008	0.144 862	0.165 612	0.190 133	0.218 867	0.252 219	0.290 188	0.331 399
0.009	0.162 994	0.186 339	0.213 927	0.246 254	0.283 775	0.326 491	0.372 855
0.010	0.181 135	0.207 075	0.237 730	0.273 651	0.315 342	0.362 804	0.414 322

Table A.30: The xz-direction (x-component and z-component) dipole moments of CO_2 at different electric fields at the MP2 level of theory for the ACCQ basis set.

XZ-Direction (X Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.007 100	0.007 728	0.008 384	0.009 060	0.009 748	0.010 440	0.011 133
0.002	0.014 324	0.015 590	0.016 913	0.018 277	0.019 665	0.021 062	0.022 458
0.003	0.021 487	0.023 386	0.025 371	0.027 417	0.029 499	0.031 595	0.033 691
0.004	0.028 652	0.031 184	0.033 832	0.036 560	0.039 336	0.042 132	0.044 927
0.005	0.035 818	0.038 984	0.042 295	0.045 706	0.049 177	0.052 673	0.056 168
0.006	0.042 987	0.046 788	0.050 761	0.054 856	0.059 023	0.063 219	0.067 414
0.007	0.050 160	0.054 594	0.059 231	0.064 010	0.068 874	0.073 772	0.078 669
0.008	0.057 336	0.062 405	0.067 706	0.073 170	0.078 731	0.084 332	0.089 931
0.009	0.064 516	0.070 220	0.076 186	0.082 337	0.088 596	0.094 901	0.101 204
0.010	0.071 700	0.078 041	0.084 673	0.091 510	0.098 470	0.105 480	0.112 488
XZ-Direction (Z Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.012 797	0.014 631	0.016 798	0.019 338	0.022 285	0.025 641	0.029 282
0.002	0.025 595	0.029 262	0.033 596	0.038 675	0.044 571	0.051 282	0.058 566
0.003	0.038 394	0.043 895	0.050 397	0.058 015	0.066 858	0.076 926	0.087 850
0.004	0.051 195	0.058 530	0.067 199	0.077 357	0.089 149	0.102 573	0.117 140
0.005	0.063 999	0.073 168	0.084 004	0.096 703	0.111 443	0.128 224	0.146 435
0.006	0.076 806	0.087 810	0.100 814	0.116 053	0.133 742	0.153 880	0.175 736
0.007	0.089 617	0.102 456	0.117 628	0.135 409	0.156 047	0.179 543	0.205 043
0.008	0.102 433	0.117 106	0.134 448	0.154 770	0.178 358	0.205 212	0.234 357
0.009	0.115 254	0.131 763	0.151 274	0.174 139	0.200 678	0.230 890	0.263 681
0.010	0.128 081	0.146 427	0.168 108	0.193 515	0.223 006	0.256 578	0.293 015

Table A.31: The x-direction and z-direction dipole moments of CO_2 at different electric fields at the MP2 level of theory for the APC3 basis set.

				X-Direction			
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.010 124	0.011 020	0.011 958	0.012 928	0.013 917	0.014 916	0.015 917
0.002	0.020 249	0.022 040	0.023 918	0.025 857	0.027 835	0.029 833	0.031 835
0.003	0.030 375	0.033 062	0.035 879	0.038 788	0.041 756	0.044 752	0.047 757
0.004	0.040 503	0.044 086	0.047 842	0.051 722	0.055 681	0.059 677	0.063 685
0.005	0.050 633	0.055 113	0.059 809	0.064 661	0.069 610	0.074 608	0.079 620
0.006	0.060 767	0.066 144	0.071 781	0.077 604	0.083 546	0.089 546	0.095 564
0.007	0.070 904	0.077 179	0.083 758	0.090 555	0.097 490	0.104 494	0.111 519
0.008	0.081 044	0.088 219	0.095 740	0.103 512	0.111 443	0.119 452	0.127 487
0.009	0.091 191	0.099 265	0.107 731	0.116 479	0.125 406	0.134 423	0.143 470
0.010	0.101 342	0.110 317	0.119 728	0.129 454	0.139 381	0.149 408	0.159 469
				Z-Direction			
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 001	0.000 000	0.000 000	0.000 000
0.001	0.018 092	0.020 683	0.023 745	0.027 335	0.031 502	0.036 246	0.041 397
0.002	0.036 185	0.041 367	0.047 492	0.054 671	0.063 005	0.072 494	0.082 796
0.003	0.054 281	0.062 054	0.071 242	0.082 009	0.094 510	0.108 745	0.124 198
0.004	0.072 379	0.082 743	0.094 994	0.109 352	0.126 019	0.144 999	0.165 605
0.005	0.090 482	0.103 438	0.118 751	0.136 699	0.157 534	0.181 259	0.207 018
0.006	0.108 590	0.124 137	0.142 515	0.164 052	0.189 055	0.217 526	0.248 438
0.007	0.126 704	0.144 844	0.166 286	0.191 414	0.220 584	0.253 801	0.289 866
0.008	0.144 825	0.165 558	0.190 064	0.218 784	0.252 123	0.290 086	0.331 305
0.009	0.162 955	0.186 282	0.213 853	0.246 164	0.283 672	0.326 382	0.372 755
0.010	0.181 094	0.207 015	0.237 653	0.273 556	0.315 233	0.362 690	0.414 220

Table A.32: The xz-direction (x-component and z-component) dipole moments of CO_2 at different electric fields at the MP2 level of theory for the APC3 basis set.

XZ-Direction (X Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000	0.000 000
0.001	0.007 098	0.007 726	0.008 384	0.009 063	0.009 757	0.010 457	0.011 159
0.002	0.014 319	0.015 585	0.016 913	0.018 284	0.019 683	0.021 095	0.022 511
0.003	0.021 479	0.023 379	0.025 371	0.027 428	0.029 527	0.031 646	0.033 770
0.004	0.028 642	0.031 175	0.033 832	0.036 575	0.039 374	0.042 201	0.045 034
0.005	0.035 806	0.038 975	0.042 295	0.045 726	0.049 226	0.052 760	0.056 304
0.006	0.042 974	0.046 777	0.050 763	0.054 882	0.059 084	0.063 327	0.067 582
0.007	0.050 146	0.054 584	0.059 236	0.064 043	0.068 948	0.073 901	0.078 868
0.008	0.057 321	0.062 395	0.067 715	0.073 211	0.078 820	0.084 485	0.090 165
0.009	0.064 502	0.070 212	0.076 199	0.082 387	0.088 702	0.095 079	0.101 475
0.010	0.071 688	0.078 036	0.084 692	0.091 571	0.098 593	0.105 685	0.112 798
XZ-Direction (Z Dipole)							
Field Strength	-18.00%	-12.00%	-6.00%	0.00%	6.00%	12.00%	18.00%
0.000	0.000 000	0.000 000	0.000 000	0.000 001	0.000 000	0.000 002	0.000 000
0.001	0.012 793	0.014 625	0.016 791	0.019 329	0.022 275	0.025 630	0.029 272
0.002	0.025 587	0.029 251	0.033 582	0.038 658	0.044 551	0.051 261	0.058 545
0.003	0.038 382	0.043 879	0.050 376	0.057 990	0.066 829	0.076 895	0.087 822
0.004	0.051 180	0.058 509	0.067 172	0.077 325	0.089 111	0.102 533	0.117 104
0.005	0.063 981	0.073 142	0.083 971	0.096 663	0.111 397	0.128 175	0.146 390
0.006	0.076 785	0.087 780	0.100 776	0.116 007	0.133 689	0.153 824	0.175 684
0.007	0.089 594	0.102 422	0.117 586	0.135 357	0.155 988	0.179 480	0.204 986
0.008	0.102 408	0.117 070	0.134 402	0.154 714	0.178 295	0.205 146	0.234 297
0.009	0.115 228	0.131 726	0.151 226	0.174 080	0.200 611	0.230 821	0.263 620
0.010	0.128 056	0.146 388	0.168 058	0.193 454	0.222 937	0.256 508	0.292 956

A.6 Root Mean Squared Error for the Fitting Functions Used to Find the Polarizabilities and Hyperpolarizabilities

Table A.33: The RMSE for the X-Direction fitting functions at a maximum field of 0.005.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.603\,57 \times 10^{-10}$	$1.649\,09 \times 10^{-7}$	1.9975×10^{-10}	$2.204\,86 \times 10^{-7}$	$5.500\,63 \times 10^{-11}$	$2.889\,45 \times 10^{-10}$
	-12.00 %	$2.801\,74 \times 10^{-11}$	$2.716\,89 \times 10^{-7}$	$1.608\,75 \times 10^{-10}$	$2.967\,46 \times 10^{-7}$	$1.992\,28 \times 10^{-10}$	$8.529\,81 \times 10^{-11}$
	-6.00 %	$4.274\,75 \times 10^{-11}$	$1.613\,37 \times 10^{-7}$	1.9869×10^{-10}	$1.559\,26 \times 10^{-7}$	$1.628\,07 \times 10^{-10}$	$4.703\,06 \times 10^{-11}$
	0.00 %	$8.257\,01 \times 10^{-11}$	$1.097\,43 \times 10^{-7}$	$1.107\,91 \times 10^{-10}$	8.6383×10^{-8}	$4.206\,01 \times 10^{-11}$	$2.512\,74 \times 10^{-10}$
	6.00 %	$1.574\,61 \times 10^{-10}$	$2.716\,89 \times 10^{-7}$	$8.392\,99 \times 10^{-11}$	$2.172\,36 \times 10^{-7}$	$1.342\,99 \times 10^{-10}$	$8.260\,87 \times 10^{-11}$
	12.00 %	$1.426\,28 \times 10^{-10}$	$2.794\,43 \times 10^{-7}$	$7.593\,85 \times 10^{-11}$	$1.575\,18 \times 10^{-7}$	$2.157\,25 \times 10^{-10}$	1.0117×10^{-10}
	18.00 %	$1.195\,62 \times 10^{-10}$	$1.880\,25 \times 10^{-7}$	$1.521\,93 \times 10^{-10}$	$1.745\,49 \times 10^{-7}$	$7.971\,88 \times 10^{-11}$	$4.717\,54 \times 10^{-11}$
ACCQ	-18.00 %	$4.765\,52 \times 10^{-11}$	$2.716\,89 \times 10^{-7}$	$1.309\,14 \times 10^{-10}$	2.106×10^{-7}	$1.006\,81 \times 10^{-10}$	1.0111×10^{-10}
	-12.00 %	$1.594\,99 \times 10^{-10}$	$1.684\,06 \times 10^{-7}$	$9.760\,72 \times 10^{-11}$	$1.558\,25 \times 10^{-7}$	$1.243\,16 \times 10^{-10}$	$5.667\,28 \times 10^{-11}$
	-6.00 %	$1.992\,29 \times 10^{-10}$	$2.695\,36 \times 10^{-7}$	1.9367×10^{-11}	$1.838\,74 \times 10^{-7}$	$8.443\,75 \times 10^{-11}$	$4.215\,09 \times 10^{-11}$
	0.00 %	$1.195\,65 \times 10^{-10}$	$1.718\,31 \times 10^{-7}$	$5.699\,66 \times 10^{-11}$	$1.840\,97 \times 10^{-7}$	$2.360\,51 \times 10^{-10}$	5.9098×10^{-11}
	6.00 %	$1.301\,97 \times 10^{-10}$	$2.373\,45 \times 10^{-7}$	$2.011\,13 \times 10^{-10}$	$1.572\,67 \times 10^{-7}$	$1.415\,59 \times 10^{-10}$	$1.194\,32 \times 10^{-10}$
	12.00 %	$2.783\,55 \times 10^{-11}$	$2.414\,02 \times 10^{-7}$	$1.553\,96 \times 10^{-10}$	$1.078\,26 \times 10^{-7}$	$1.810\,07 \times 10^{-10}$	$1.970\,03 \times 10^{-10}$
	18.00 %	$1.096\,08 \times 10^{-10}$	$2.508\,73 \times 10^{-7}$	6.1511×10^{-11}	$7.163\,49 \times 10^{-8}$	$1.345\,14 \times 10^{-10}$	$5.950\,19 \times 10^{-11}$
APC3	-18.00 %	2.303×10^{-11}	$1.613\,37 \times 10^{-7}$	$5.631\,92 \times 10^{-9}$	$1.455\,58 \times 10^{-7}$	$5.385\,17 \times 10^{-9}$	$6.516\,87 \times 10^{-9}$
	-12.00 %	$1.218\,28 \times 10^{-10}$	$1.684\,06 \times 10^{-7}$	1.12×10^{-9}	$2.246\,35 \times 10^{-7}$	$1.513\,11 \times 10^{-9}$	$1.480\,23 \times 10^{-9}$
	-6.00 %	$1.594\,53 \times 10^{-10}$	$2.315\,45 \times 10^{-7}$	1.6235×10^{-9}	$1.333\,12 \times 10^{-7}$	$1.207\,61 \times 10^{-9}$	$3.364\,06 \times 10^{-9}$
	0.00 %	$8.175\,39 \times 10^{-11}$	$2.373\,45 \times 10^{-7}$	$1.970\,84 \times 10^{-10}$	$9.922\,28 \times 10^{-8}$	$2.884\,06 \times 10^{-10}$	6.2411×10^{-10}
	6.00 %	$5.735\,02 \times 10^{-11}$	$1.132\,28 \times 10^{-7}$	$4.844\,25 \times 10^{-10}$	$1.260\,29 \times 10^{-7}$	$4.321\,24 \times 10^{-10}$	$5.960\,24 \times 10^{-10}$
	12.00 %	$1.446\,89 \times 10^{-10}$	$1.448\,41 \times 10^{-7}$	$1.910\,72 \times 10^{-10}$	$8.212\,23 \times 10^{-8}$	$2.825\,91 \times 10^{-10}$	$3.451\,84 \times 10^{-10}$
	18.00 %	$1.295\,57 \times 10^{-10}$	$2.599\,98 \times 10^{-7}$	$1.956\,14 \times 10^{-10}$	$1.885\,79 \times 10^{-7}$	$2.227\,41 \times 10^{-10}$	$2.069\,69 \times 10^{-10}$

Table A.34: The RMSE for the X-Direction fitting functions at a maximum field of 0.01.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.347\,45 \times 10^{-10}$	$2.464\,21 \times 10^{-7}$	$1.348\,11 \times 10^{-10}$	2.8127×10^{-7}	$1.356\,63 \times 10^{-10}$	$4.023\,89 \times 10^{-10}$
	-12.00 %	$5.649\,46 \times 10^{-11}$	$2.654\,59 \times 10^{-7}$	$3.294\,47 \times 10^{-11}$	$1.203\,23 \times 10^{-7}$	$2.096\,06 \times 10^{-10}$	$1.311\,16 \times 10^{-10}$
	-6.00 %	$1.068\,59 \times 10^{-10}$	$2.558\,59 \times 10^{-7}$	9.2712×10^{-11}	$2.165\,45 \times 10^{-7}$	$6.659\,91 \times 10^{-10}$	$1.307\,12 \times 10^{-9}$
	0.00 %	$1.020\,85 \times 10^{-10}$	$2.489\,66 \times 10^{-7}$	1.2513×10^{-10}	$1.255\,07 \times 10^{-7}$	$1.560\,15 \times 10^{-10}$	$7.552\,53 \times 10^{-11}$
	6.00 %	$1.599\,78 \times 10^{-10}$	$2.230\,33 \times 10^{-7}$	$6.257\,14 \times 10^{-11}$	$1.432\,95 \times 10^{-7}$	$2.003\,57 \times 10^{-10}$	$1.301\,03 \times 10^{-10}$
	12.00 %	$5.265\,78 \times 10^{-11}$	$3.256\,35 \times 10^{-7}$	$8.616\,96 \times 10^{-11}$	$1.846\,32 \times 10^{-7}$	$1.658\,04 \times 10^{-10}$	$1.361\,45 \times 10^{-9}$
	18.00 %	$6.118\,56 \times 10^{-11}$	$1.694\,28 \times 10^{-7}$	1.2658×10^{-10}	$2.010\,05 \times 10^{-7}$	$3.976\,06 \times 10^{-9}$	$4.663\,15 \times 10^{-9}$
ACCQ	-18.00 %	$1.666\,04 \times 10^{-10}$	$2.407\,14 \times 10^{-7}$	$2.109\,56 \times 10^{-10}$	$1.541\,91 \times 10^{-7}$	$1.836\,92 \times 10^{-10}$	$9.599\,33 \times 10^{-11}$
	-12.00 %	$6.918\,48 \times 10^{-11}$	$2.424\,14 \times 10^{-7}$	$1.072\,13 \times 10^{-10}$	$1.733\,56 \times 10^{-7}$	$4.968\,14 \times 10^{-11}$	$1.186\,24 \times 10^{-10}$
	-6.00 %	$6.958\,78 \times 10^{-11}$	2.4397×10^{-7}	$1.806\,74 \times 10^{-10}$	$2.536\,04 \times 10^{-7}$	$5.151\,77 \times 10^{-10}$	$1.184\,49 \times 10^{-9}$
	0.00 %	$1.609\,32 \times 10^{-10}$	$2.212\,39 \times 10^{-7}$	$9.636\,62 \times 10^{-11}$	$1.209\,59 \times 10^{-7}$	$1.654\,34 \times 10^{-10}$	$8.673\,01 \times 10^{-11}$
	6.00 %	$1.555\,28 \times 10^{-10}$	2.6713×10^{-7}	$1.030\,61 \times 10^{-10}$	$1.249\,61 \times 10^{-7}$	$1.484\,95 \times 10^{-10}$	$1.291\,57 \times 10^{-10}$
	12.00 %	$1.650\,99 \times 10^{-10}$	$1.875\,89 \times 10^{-7}$	$9.104\,28 \times 10^{-11}$	9.5862×10^{-8}	$1.380\,33 \times 10^{-10}$	$1.716\,76 \times 10^{-10}$
	18.00 %	$1.237\,98 \times 10^{-10}$	$2.527\,27 \times 10^{-7}$	$1.153\,27 \times 10^{-10}$	$2.108\,68 \times 10^{-7}$	$3.786\,24 \times 10^{-9}$	$5.625\,75 \times 10^{-9}$
APC3	-18.00 %	$3.563\,53 \times 10^{-11}$	$2.055\,39 \times 10^{-7}$	$7.632\,49 \times 10^{-9}$	$1.478\,69 \times 10^{-7}$	$8.001\,91 \times 10^{-9}$	$1.892\,32 \times 10^{-8}$
	-12.00 %	$6.788\,96 \times 10^{-11}$	$2.142\,75 \times 10^{-7}$	$2.916\,72 \times 10^{-9}$	1.1796×10^{-7}	$2.693\,37 \times 10^{-9}$	$3.302\,97 \times 10^{-9}$
	-6.00 %	$1.074\,94 \times 10^{-10}$	$2.528\,44 \times 10^{-7}$	$1.467\,99 \times 10^{-9}$	$1.201\,12 \times 10^{-7}$	$1.132\,86 \times 10^{-9}$	$2.838\,11 \times 10^{-9}$
	0.00 %	$7.547\,81 \times 10^{-11}$	$1.943\,36 \times 10^{-7}$	5.0066×10^{-10}	$1.520\,04 \times 10^{-7}$	$4.264\,82 \times 10^{-10}$	$6.226\,37 \times 10^{-10}$
	6.00 %	$1.826\,72 \times 10^{-10}$	$2.392\,96 \times 10^{-7}$	5.4627×10^{-10}	1.353×10^{-7}	$6.205\,59 \times 10^{-10}$	$7.213\,17 \times 10^{-10}$
	12.00 %	$6.826\,09 \times 10^{-11}$	$2.039\,62 \times 10^{-7}$	$2.829\,33 \times 10^{-10}$	$2.175\,41 \times 10^{-7}$	$3.052\,07 \times 10^{-10}$	$3.770\,74 \times 10^{-10}$
	18.00 %	$9.655\,72 \times 10^{-11}$	$2.459\,71 \times 10^{-7}$	$1.867\,09 \times 10^{-10}$	$1.923\,75 \times 10^{-7}$	$2.805\,22 \times 10^{-10}$	$2.798\,57 \times 10^{-10}$

Table A.35: The RMSE for the X-Direction fitting functions at a maximum field of 0.015.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$9.022\,01 \times 10^{-10}$	4.5486×10^{-10}	$1.281\,61 \times 10^{-9}$	$8.191\,87 \times 10^{-10}$
	-12.00 %	$5.248\,93 \times 10^{-10}$	1.3201×10^{-9}	4.0195×10^{-10}	$9.639\,87 \times 10^{-10}$
	-6.00 %	$4.430\,28 \times 10^{-10}$	$4.450\,75 \times 10^{-10}$	$1.645\,72 \times 10^{-9}$	$2.243\,38 \times 10^{-9}$
	0.00 %	$1.090\,61 \times 10^{-9}$	$4.094\,84 \times 10^{-10}$	$9.962\,82 \times 10^{-10}$	$9.562\,44 \times 10^{-10}$
	6.00 %	$3.573\,02 \times 10^{-10}$	4.1294×10^{-10}	$1.401\,35 \times 10^{-9}$	2.9622×10^{-10}
	12.00 %	$7.280\,06 \times 10^{-10}$	$6.799\,32 \times 10^{-10}$	$8.315\,05 \times 10^{-10}$	$1.662\,51 \times 10^{-9}$
	18.00 %	$2.135\,36 \times 10^{-10}$	$4.734\,81 \times 10^{-10}$	$3.871\,84 \times 10^{-9}$	$4.465\,61 \times 10^{-9}$
ACCQ	-18.00 %	$6.280\,92 \times 10^{-10}$	1.0429×10^{-9}	$1.772\,42 \times 10^{-10}$	5.2049×10^{-10}
	-12.00 %	$4.343\,35 \times 10^{-10}$	$7.738\,69 \times 10^{-10}$	$5.836\,15 \times 10^{-10}$	$1.008\,44 \times 10^{-9}$
	-6.00 %	$4.135\,17 \times 10^{-10}$	$1.330\,18 \times 10^{-10}$	$1.240\,35 \times 10^{-9}$	$1.705\,25 \times 10^{-9}$
	0.00 %	$8.315\,08 \times 10^{-10}$	$8.698\,49 \times 10^{-10}$	$1.249\,95 \times 10^{-9}$	$4.450\,06 \times 10^{-10}$
	6.00 %	$9.720\,03 \times 10^{-10}$	$3.558\,64 \times 10^{-10}$	$3.646\,31 \times 10^{-10}$	8.3573×10^{-10}
	12.00 %	$7.802\,49 \times 10^{-10}$	$2.959\,77 \times 10^{-10}$	3.45×10^{-10}	$8.027\,67 \times 10^{-10}$
	18.00 %	$5.450\,94 \times 10^{-10}$	$3.497\,52 \times 10^{-10}$	$4.488\,08 \times 10^{-9}$	$6.567\,41 \times 10^{-9}$
APC3	-18.00 %	1.6319×10^{-10}	$8.759\,35 \times 10^{-9}$	$8.103\,67 \times 10^{-9}$	$1.821\,15 \times 10^{-8}$
	-12.00 %	$6.747\,53 \times 10^{-10}$	$3.070\,39 \times 10^{-9}$	$3.022\,41 \times 10^{-9}$	$3.311\,86 \times 10^{-9}$
	-6.00 %	$1.140\,59 \times 10^{-9}$	$1.844\,14 \times 10^{-9}$	$1.864\,43 \times 10^{-9}$	$2.724\,63 \times 10^{-9}$
	0.00 %	4.2045×10^{-10}	$1.304\,08 \times 10^{-9}$	8.4754×10^{-10}	1.3608×10^{-9}
	6.00 %	$7.965\,77 \times 10^{-10}$	7.1153×10^{-10}	$6.178\,63 \times 10^{-10}$	$1.298\,92 \times 10^{-9}$
	12.00 %	$9.116\,27 \times 10^{-10}$	$1.033\,12 \times 10^{-9}$	$5.799\,85 \times 10^{-10}$	$7.638\,51 \times 10^{-10}$
	18.00 %	$1.122\,42 \times 10^{-9}$	$7.405\,21 \times 10^{-10}$	$7.910\,02 \times 10^{-10}$	$8.057\,93 \times 10^{-10}$

Table A.36: The RMSE for the X-Direction fitting functions at a maximum field of 0.02.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.042\,31 \times 10^{-9}$	$1.046\,73 \times 10^{-9}$	$1.103\,22 \times 10^{-9}$	$1.119\,87 \times 10^{-9}$
	-12.00 %	$6.906\,05 \times 10^{-10}$	$1.247\,54 \times 10^{-9}$	1.4774×10^{-9}	$8.323\,24 \times 10^{-10}$
	-6.00 %	$7.972\,19 \times 10^{-10}$	$7.794\,43 \times 10^{-10}$	$1.396\,58 \times 10^{-9}$	$2.369\,08 \times 10^{-9}$
	0.00 %	1.2687×10^{-9}	$1.063\,23 \times 10^{-9}$	$1.472\,66 \times 10^{-9}$	$1.214\,99 \times 10^{-9}$
	6.00 %	$1.604\,49 \times 10^{-9}$	$1.339\,45 \times 10^{-9}$	$1.677\,05 \times 10^{-9}$	$1.706\,04 \times 10^{-9}$
	12.00 %	$1.524\,83 \times 10^{-9}$	$2.196\,67 \times 10^{-9}$	$1.888\,29 \times 10^{-9}$	$2.993\,16 \times 10^{-9}$
	18.00 %	$1.486\,43 \times 10^{-9}$	$2.251\,38 \times 10^{-9}$	$5.709\,69 \times 10^{-9}$	$6.610\,72 \times 10^{-9}$
ACCQ	-18.00 %	$9.996\,26 \times 10^{-10}$	$1.438\,82 \times 10^{-9}$	$1.113\,84 \times 10^{-9}$	$1.563\,83 \times 10^{-9}$
	-12.00 %	$1.204\,99 \times 10^{-9}$	$8.888\,31 \times 10^{-10}$	$7.843\,78 \times 10^{-10}$	$1.614\,37 \times 10^{-9}$
	-6.00 %	$1.309\,61 \times 10^{-9}$	$1.052\,69 \times 10^{-9}$	$1.201\,99 \times 10^{-9}$	$1.572\,13 \times 10^{-9}$
	0.00 %	1.209×10^{-9}	$1.543\,97 \times 10^{-9}$	$1.528\,57 \times 10^{-9}$	$1.399\,69 \times 10^{-9}$
	6.00 %	$1.632\,72 \times 10^{-9}$	$2.267\,09 \times 10^{-9}$	$1.576\,22 \times 10^{-9}$	$2.014\,37 \times 10^{-9}$
	12.00 %	$1.539\,09 \times 10^{-9}$	$2.494\,06 \times 10^{-9}$	$2.263\,59 \times 10^{-9}$	$2.744\,29 \times 10^{-9}$
	18.00 %	$2.159\,06 \times 10^{-9}$	$3.178\,81 \times 10^{-9}$	4.3999×10^{-9}	6.785×10^{-9}
APC3	-18.00 %	$1.330\,88 \times 10^{-9}$	$8.480\,94 \times 10^{-9}$	$8.036\,89 \times 10^{-9}$	$1.747\,06 \times 10^{-8}$
	-12.00 %	$1.675\,56 \times 10^{-9}$	$3.502\,26 \times 10^{-9}$	$3.188\,34 \times 10^{-9}$	$4.691\,97 \times 10^{-9}$
	-6.00 %	$1.953\,05 \times 10^{-9}$	$2.686\,63 \times 10^{-9}$	$2.141\,75 \times 10^{-9}$	$3.092\,76 \times 10^{-9}$
	0.00 %	$1.605\,86 \times 10^{-9}$	$2.646\,72 \times 10^{-9}$	$2.182\,29 \times 10^{-9}$	$2.847\,11 \times 10^{-9}$
	6.00 %	$2.144\,05 \times 10^{-9}$	$3.239\,97 \times 10^{-9}$	$2.839\,64 \times 10^{-9}$	3.3983×10^{-9}
	12.00 %	$2.485\,44 \times 10^{-9}$	$4.188\,77 \times 10^{-9}$	$3.516\,57 \times 10^{-9}$	$4.310\,76 \times 10^{-9}$
	18.00 %	$2.875\,04 \times 10^{-9}$	$5.666\,52 \times 10^{-9}$	$4.590\,27 \times 10^{-9}$	$5.488\,33 \times 10^{-9}$

Table A.37: The RMSE for the Z-Direction fitting functions at a maximum field of 0.005.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.284\,56 \times 10^{-10}$	$2.695\,36 \times 10^{-7}$	$1.380\,29 \times 10^{-9}$	$1.992\,79 \times 10^{-7}$	$1.484\,21 \times 10^{-10}$	$5.548\,72 \times 10^{-10}$
	-12.00 %	$2.054\,97 \times 10^{-10}$	$1.684\,06 \times 10^{-7}$	$7.974\,41 \times 10^{-10}$	$1.060\,92 \times 10^{-7}$	$1.698\,29 \times 10^{-10}$	$8.996\,84 \times 10^{-11}$
	-6.00 %	1.8236×10^{-10}	$3.520\,39 \times 10^{-7}$	$3.928\,06 \times 10^{-9}$	$1.441\,56 \times 10^{-7}$	$1.343\,29 \times 10^{-10}$	$1.222\,15 \times 10^{-10}$
	0.00 %	$8.245\,12 \times 10^{-11}$	$3.729\,39 \times 10^{-7}$	6.4984×10^{-9}	$2.864\,22 \times 10^{-7}$	$9.196\,03 \times 10^{-10}$	$3.766\,34 \times 10^{-10}$
	6.00 %	1.92×10^{-10}	$3.760\,51 \times 10^{-7}$	$4.685\,99 \times 10^{-10}$	$2.193\,35 \times 10^{-7}$	$1.779\,01 \times 10^{-9}$	$5.111\,46 \times 10^{-10}$
	12.00 %	$3.995\,37 \times 10^{-11}$	$5.746\,52 \times 10^{-7}$	$4.112\,78 \times 10^{-9}$	$2.764\,33 \times 10^{-7}$	$4.344\,94 \times 10^{-9}$	$2.720\,02 \times 10^{-9}$
	18.00 %	$1.445\,43 \times 10^{-10}$	$1.132\,28 \times 10^{-7}$	2.9085×10^{-8}	$6.096\,42 \times 10^{-7}$	$6.226\,04 \times 10^{-9}$	$6.788\,63 \times 10^{-9}$
ACCQ	-18.00 %	$8.162\,41 \times 10^{-11}$	$2.422\,06 \times 10^{-7}$	$1.368\,17 \times 10^{-9}$	$2.162\,16 \times 10^{-7}$	2.2395×10^{-10}	$1.039\,27 \times 10^{-10}$
	-12.00 %	$1.943\,46 \times 10^{-10}$	$1.718\,31 \times 10^{-7}$	$1.934\,89 \times 10^{-9}$	$1.438\,47 \times 10^{-7}$	$2.019\,48 \times 10^{-10}$	$2.130\,08 \times 10^{-10}$
	-6.00 %	$1.468\,91 \times 10^{-11}$	2.446×10^{-7}	$1.387\,04 \times 10^{-9}$	$2.605\,83 \times 10^{-7}$	2.0797×10^{-10}	$8.778\,76 \times 10^{-11}$
	0.00 %	1.2286×10^{-10}	$1.649\,09 \times 10^{-7}$	$9.401\,46 \times 10^{-9}$	$2.180\,45 \times 10^{-7}$	$1.095\,43 \times 10^{-9}$	$3.536\,21 \times 10^{-10}$
	6.00 %	$1.543\,56 \times 10^{-10}$	$2.194\,86 \times 10^{-7}$	$6.889\,61 \times 10^{-10}$	$8.356\,38 \times 10^{-8}$	$1.745\,24 \times 10^{-9}$	$6.164\,87 \times 10^{-10}$
	12.00 %	1.2562×10^{-10}	4.7469×10^{-7}	$4.629\,77 \times 10^{-9}$	$2.544\,15 \times 10^{-7}$	$6.390\,83 \times 10^{-9}$	$7.860\,13 \times 10^{-9}$
	18.00 %	$2.162\,23 \times 10^{-10}$	$2.194\,86 \times 10^{-7}$	$2.967\,75 \times 10^{-8}$	$6.224\,75 \times 10^{-7}$	$5.548\,83 \times 10^{-9}$	9.7428×10^{-9}
APC3	-18.00 %	1.4074×10^{-10}	$8.591\,57 \times 10^{-8}$	$1.859\,46 \times 10^{-9}$	$1.592\,78 \times 10^{-7}$	$2.065\,42 \times 10^{-10}$	$1.350\,55 \times 10^{-10}$
	-12.00 %	$2.197\,93 \times 10^{-10}$	$2.194\,86 \times 10^{-7}$	$2.677\,46 \times 10^{-9}$	$1.946\,86 \times 10^{-7}$	$2.636\,18 \times 10^{-10}$	$2.479\,98 \times 10^{-10}$
	-6.00 %	$1.221\,52 \times 10^{-10}$	$2.194\,86 \times 10^{-7}$	$4.067\,81 \times 10^{-10}$	$1.813\,05 \times 10^{-7}$	$2.360\,52 \times 10^{-10}$	$2.327\,41 \times 10^{-10}$
	0.00 %	$1.375\,89 \times 10^{-10}$	$3.729\,39 \times 10^{-7}$	$4.922\,73 \times 10^{-9}$	$3.593\,75 \times 10^{-7}$	$2.137\,22 \times 10^{-10}$	$1.132\,28 \times 10^{-10}$
	6.00 %	$2.285\,01 \times 10^{-10}$	$1.961\,16 \times 10^{-7}$	$3.864\,58 \times 10^{-9}$	$2.078\,87 \times 10^{-7}$	$4.304\,69 \times 10^{-10}$	$2.105\,68 \times 10^{-10}$
	12.00 %	$2.239\,54 \times 10^{-10}$	$1.990\,65 \times 10^{-7}$	$6.249\,86 \times 10^{-10}$	$1.286\,31 \times 10^{-7}$	$7.426\,72 \times 10^{-9}$	$7.315\,57 \times 10^{-9}$
	18.00 %	$1.597\,95 \times 10^{-10}$	$2.716\,89 \times 10^{-7}$	$5.444\,18 \times 10^{-9}$	$2.668\,55 \times 10^{-7}$	$5.308\,75 \times 10^{-9}$	$9.155\,54 \times 10^{-9}$

Table A.38: The RMSE for the Z-Direction fitting functions at a maximum field of 0.01.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.503\,75 \times 10^{-10}$	$2.935\,51 \times 10^{-7}$	$1.321\,63 \times 10^{-9}$	1.8124×10^{-7}	$1.545\,04 \times 10^{-10}$	$8.094\,65 \times 10^{-10}$
	-12.00 %	$2.295\,65 \times 10^{-10}$	$4.366\,89 \times 10^{-7}$	$1.339\,95 \times 10^{-9}$	$9.814\,39 \times 10^{-8}$	$1.273\,19 \times 10^{-9}$	$1.004\,65 \times 10^{-9}$
	-6.00 %	$5.363\,86 \times 10^{-10}$	$7.286\,52 \times 10^{-7}$	$5.203\,96 \times 10^{-9}$	$1.173\,66 \times 10^{-7}$	$1.208\,44 \times 10^{-9}$	$6.298\,69 \times 10^{-10}$
	0.00 %	$1.250\,16 \times 10^{-9}$	$3.153\,77 \times 10^{-7}$	$6.192\,62 \times 10^{-9}$	$2.218\,67 \times 10^{-7}$	$1.817\,83 \times 10^{-9}$	$1.163\,07 \times 10^{-9}$
	6.00 %	$9.683\,47 \times 10^{-10}$	$3.384\,46 \times 10^{-7}$	$1.718\,96 \times 10^{-9}$	1.0767×10^{-7}	$2.233\,88 \times 10^{-9}$	$8.125\,05 \times 10^{-10}$
	12.00 %	$2.969\,95 \times 10^{-10}$	$4.973\,19 \times 10^{-7}$	$4.178\,21 \times 10^{-9}$	2.0801×10^{-7}	$7.345\,93 \times 10^{-9}$	3.7098×10^{-9}
	18.00 %	$5.197\,93 \times 10^{-10}$	$5.502\,11 \times 10^{-7}$	4.0742×10^{-8}	1.1319×10^{-6}	$4.910\,94 \times 10^{-9}$	$6.179\,88 \times 10^{-9}$
ACCQ	-18.00 %	$1.266\,59 \times 10^{-10}$	$3.227\,25 \times 10^{-7}$	$1.661\,01 \times 10^{-9}$	$1.680\,21 \times 10^{-7}$	$1.294\,25 \times 10^{-10}$	8.4306×10^{-11}
	-12.00 %	$4.260\,08 \times 10^{-11}$	$2.086\,64 \times 10^{-7}$	$1.737\,79 \times 10^{-9}$	$1.309\,81 \times 10^{-7}$	$1.144\,36 \times 10^{-9}$	$8.928\,86 \times 10^{-10}$
	-6.00 %	$1.245\,23 \times 10^{-9}$	$5.658\,52 \times 10^{-7}$	$3.118\,52 \times 10^{-9}$	$2.755\,35 \times 10^{-7}$	$6.451\,96 \times 10^{-10}$	$1.052\,67 \times 10^{-9}$
	0.00 %	$6.477\,02 \times 10^{-10}$	$2.704\,16 \times 10^{-7}$	$7.141\,37 \times 10^{-9}$	$2.473\,72 \times 10^{-7}$	$1.211\,13 \times 10^{-9}$	$9.465\,14 \times 10^{-10}$
	6.00 %	$1.626\,45 \times 10^{-10}$	$3.283\,74 \times 10^{-7}$	$2.103\,99 \times 10^{-9}$	$2.432\,66 \times 10^{-7}$	$2.206\,73 \times 10^{-9}$	$1.171\,84 \times 10^{-9}$
	12.00 %	$4.127\,92 \times 10^{-10}$	$5.035\,54 \times 10^{-7}$	$4.333\,24 \times 10^{-9}$	$2.284\,94 \times 10^{-7}$	$5.798\,83 \times 10^{-9}$	$7.296\,33 \times 10^{-9}$
	18.00 %	$1.796\,26 \times 10^{-10}$	$3.693\,86 \times 10^{-7}$	$4.130\,99 \times 10^{-8}$	$1.085\,99 \times 10^{-6}$	$4.200\,98 \times 10^{-9}$	$8.006\,55 \times 10^{-9}$
APC3	-18.00 %	$7.720\,68 \times 10^{-11}$	$3.023\,51 \times 10^{-7}$	1.694×10^{-9}	$2.020\,52 \times 10^{-7}$	$2.831\,37 \times 10^{-10}$	$1.729\,84 \times 10^{-10}$
	-12.00 %	$9.468\,04 \times 10^{-11}$	$2.387\,93 \times 10^{-7}$	2.4342×10^{-9}	$1.531\,43 \times 10^{-7}$	$8.545\,04 \times 10^{-10}$	$5.681\,71 \times 10^{-10}$
	-6.00 %	$2.877\,74 \times 10^{-10}$	$2.465\,24 \times 10^{-7}$	$1.023\,01 \times 10^{-9}$	$2.039\,43 \times 10^{-7}$	$7.968\,76 \times 10^{-10}$	$3.001\,94 \times 10^{-10}$
	0.00 %	6.3638×10^{-10}	$3.309\,25 \times 10^{-7}$	$4.490\,72 \times 10^{-9}$	$3.344\,74 \times 10^{-7}$	$1.646\,65 \times 10^{-9}$	$7.595\,75 \times 10^{-10}$
	6.00 %	$2.402\,72 \times 10^{-10}$	$2.410\,13 \times 10^{-7}$	$3.131\,31 \times 10^{-9}$	$2.422\,47 \times 10^{-7}$	$7.001\,46 \times 10^{-10}$	$3.548\,28 \times 10^{-10}$
	12.00 %	$4.437\,57 \times 10^{-10}$	$3.653\,22 \times 10^{-7}$	1.9528×10^{-9}	$2.394\,91 \times 10^{-7}$	$6.861\,66 \times 10^{-9}$	6.7822×10^{-9}
	18.00 %	$1.151\,27 \times 10^{-9}$	$5.010\,51 \times 10^{-7}$	$1.372\,52 \times 10^{-8}$	$4.270\,04 \times 10^{-7}$	$4.077\,94 \times 10^{-9}$	$7.073\,85 \times 10^{-9}$

Table A.39: The RMSE for the Z-Direction fitting functions at a maximum field of 0.015.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$9.982\,39 \times 10^{-10}$	$1.825\,48 \times 10^{-9}$	$1.827\,67 \times 10^{-10}$	$8.467\,85 \times 10^{-10}$
	-12.00 %	$1.010\,04 \times 10^{-9}$	$1.741\,32 \times 10^{-9}$	$1.222\,69 \times 10^{-9}$	$1.554\,38 \times 10^{-9}$
	-6.00 %	$7.668\,47 \times 10^{-10}$	$5.078\,78 \times 10^{-9}$	1.457×10^{-9}	$4.756\,44 \times 10^{-10}$
	0.00 %	$7.185\,92 \times 10^{-10}$	$6.042\,74 \times 10^{-9}$	$1.953\,93 \times 10^{-9}$	$1.269\,72 \times 10^{-9}$
	6.00 %	$7.572\,63 \times 10^{-10}$	$2.089\,35 \times 10^{-9}$	$2.311\,27 \times 10^{-9}$	$1.031\,61 \times 10^{-9}$
	12.00 %	$4.435\,95 \times 10^{-10}$	$4.889\,37 \times 10^{-9}$	$7.093\,34 \times 10^{-9}$	$3.728\,15 \times 10^{-9}$
	18.00 %	$7.092\,04 \times 10^{-10}$	$4.390\,69 \times 10^{-8}$	$4.798\,65 \times 10^{-9}$	$6.394\,94 \times 10^{-9}$
ACCQ	-18.00 %	9.9609×10^{-10}	2.0037×10^{-9}	$8.638\,41 \times 10^{-10}$	$3.142\,93 \times 10^{-10}$
	-12.00 %	$1.294\,85 \times 10^{-9}$	$2.440\,16 \times 10^{-9}$	$9.740\,29 \times 10^{-10}$	$1.131\,69 \times 10^{-9}$
	-6.00 %	1.5187×10^{-9}	3.7633×10^{-9}	$1.414\,48 \times 10^{-9}$	$6.238\,18 \times 10^{-10}$
	0.00 %	$4.102\,62 \times 10^{-10}$	$7.189\,24 \times 10^{-9}$	$1.804\,33 \times 10^{-9}$	$1.193\,79 \times 10^{-9}$
	6.00 %	$7.922\,86 \times 10^{-10}$	$2.639\,12 \times 10^{-9}$	$2.578\,97 \times 10^{-9}$	$1.066\,13 \times 10^{-9}$
	12.00 %	$1.005\,41 \times 10^{-9}$	$5.664\,86 \times 10^{-9}$	$5.554\,32 \times 10^{-9}$	$6.980\,55 \times 10^{-9}$
	18.00 %	$3.343\,96 \times 10^{-10}$	$4.446\,68 \times 10^{-8}$	$4.111\,29 \times 10^{-9}$	$7.861\,16 \times 10^{-9}$
APC3	-18.00 %	$2.579\,73 \times 10^{-10}$	$1.719\,27 \times 10^{-9}$	$5.998\,06 \times 10^{-10}$	$1.394\,81 \times 10^{-9}$
	-12.00 %	3.3483×10^{-10}	$2.983\,19 \times 10^{-9}$	$7.658\,37 \times 10^{-10}$	$1.537\,62 \times 10^{-9}$
	-6.00 %	$3.531\,21 \times 10^{-10}$	$1.819\,69 \times 10^{-9}$	$7.637\,22 \times 10^{-10}$	$1.482\,58 \times 10^{-9}$
	0.00 %	$5.487\,49 \times 10^{-10}$	$4.371\,08 \times 10^{-9}$	$1.775\,98 \times 10^{-9}$	$6.876\,83 \times 10^{-10}$
	6.00 %	$7.070\,98 \times 10^{-10}$	$3.132\,44 \times 10^{-9}$	$1.376\,76 \times 10^{-9}$	$1.600\,24 \times 10^{-9}$
	12.00 %	$4.148\,12 \times 10^{-10}$	$1.707\,49 \times 10^{-9}$	$6.614\,89 \times 10^{-9}$	$6.473\,12 \times 10^{-9}$
	18.00 %	$7.629\,61 \times 10^{-10}$	$2.771\,96 \times 10^{-8}$	$4.110\,76 \times 10^{-9}$	$6.769\,17 \times 10^{-9}$

Table A.40: The RMSE for the Z-Direction fitting functions at a maximum field of 0.02.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$9.687\,18 \times 10^{-10}$	$1.608\,37 \times 10^{-9}$	$1.465\,49 \times 10^{-9}$	$1.472\,26 \times 10^{-9}$
	-12.00 %	$1.327\,59 \times 10^{-9}$	$1.700\,72 \times 10^{-9}$	$2.268\,07 \times 10^{-9}$	$2.277\,68 \times 10^{-9}$
	-6.00 %	$9.339\,51 \times 10^{-10}$	$5.563\,33 \times 10^{-9}$	$2.357\,38 \times 10^{-9}$	2.0295×10^{-9}
	0.00 %	$1.552\,99 \times 10^{-9}$	$6.975\,57 \times 10^{-9}$	3.0219×10^{-9}	$3.044\,33 \times 10^{-9}$
	6.00 %	$1.706\,66 \times 10^{-9}$	$3.853\,97 \times 10^{-9}$	$2.591\,83 \times 10^{-9}$	$2.945\,21 \times 10^{-9}$
	12.00 %	$1.714\,02 \times 10^{-9}$	$7.248\,93 \times 10^{-9}$	7.4414×10^{-9}	5.9873×10^{-9}
	18.00 %	$1.855\,06 \times 10^{-9}$	$4.577\,73 \times 10^{-8}$	$4.783\,43 \times 10^{-9}$	$6.177\,71 \times 10^{-9}$
ACCQ	-18.00 %	$1.281\,55 \times 10^{-9}$	$2.176\,82 \times 10^{-9}$	$1.736\,74 \times 10^{-9}$	$1.877\,76 \times 10^{-9}$
	-12.00 %	$1.700\,92 \times 10^{-9}$	$2.686\,49 \times 10^{-9}$	$1.874\,68 \times 10^{-9}$	$2.329\,53 \times 10^{-9}$
	-6.00 %	1.868×10^{-9}	$3.640\,12 \times 10^{-9}$	$2.876\,36 \times 10^{-9}$	$2.535\,44 \times 10^{-9}$
	0.00 %	$1.718\,25 \times 10^{-9}$	8.339×10^{-9}	$3.618\,58 \times 10^{-9}$	$3.906\,12 \times 10^{-9}$
	6.00 %	$1.704\,39 \times 10^{-9}$	$5.562\,19 \times 10^{-9}$	$2.891\,28 \times 10^{-9}$	3.6829×10^{-9}
	12.00 %	$2.040\,15 \times 10^{-9}$	$5.599\,51 \times 10^{-9}$	$6.567\,99 \times 10^{-9}$	7.6175×10^{-9}
	18.00 %	$2.285\,24 \times 10^{-9}$	$4.632\,43 \times 10^{-8}$	$4.882\,77 \times 10^{-9}$	$8.059\,98 \times 10^{-9}$
APC3	-18.00 %	$1.526\,51 \times 10^{-9}$	$3.711\,35 \times 10^{-9}$	$2.552\,92 \times 10^{-9}$	2.8247×10^{-9}
	-12.00 %	$1.866\,48 \times 10^{-9}$	$6.132\,11 \times 10^{-9}$	$2.819\,34 \times 10^{-9}$	$4.149\,26 \times 10^{-9}$
	-6.00 %	$1.971\,82 \times 10^{-9}$	5.3868×10^{-9}	$3.796\,94 \times 10^{-9}$	$4.484\,14 \times 10^{-9}$
	0.00 %	$2.506\,48 \times 10^{-9}$	$5.284\,87 \times 10^{-9}$	$6.489\,41 \times 10^{-9}$	$6.203\,99 \times 10^{-9}$
	6.00 %	$2.873\,01 \times 10^{-9}$	$6.677\,57 \times 10^{-9}$	$4.649\,63 \times 10^{-9}$	$6.168\,13 \times 10^{-9}$
	12.00 %	$3.103\,51 \times 10^{-9}$	$5.720\,91 \times 10^{-9}$	$9.418\,14 \times 10^{-9}$	$1.013\,99 \times 10^{-8}$
	18.00 %	3.7979×10^{-9}	$2.746\,77 \times 10^{-8}$	$7.600\,15 \times 10^{-9}$	1.0195×10^{-8}

Table A.41: The RMSE for the XZ-Direction fitting functions at a maximum field of 0.005.

Basis Set	Bond Length (%)	RHF Energy	RHF X Dipole	RHF Z Dipole	MP2 Energy	MP2 X Dipole	MP2 Z Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.640\,81 \times 10^{-8}$	$2.114\,96 \times 10^{-7}$	$1.095\,74 \times 10^{-7}$	$1.576\,89 \times 10^{-8}$	$2.339\,29 \times 10^{-5}$	2.6145×10^{-7}	$1.712\,39 \times 10^{-8}$	$1.772\,04 \times 10^{-8}$
	-12.00 %	$1.787\,32 \times 10^{-8}$	$1.612\,44 \times 10^{-7}$	$3.519\,99 \times 10^{-7}$	$1.959\,46 \times 10^{-8}$	$2.534\,69 \times 10^{-5}$	$1.876\,87 \times 10^{-7}$	$1.886\,45 \times 10^{-8}$	$1.862\,59 \times 10^{-8}$
	-6.00 %	$1.933\,81 \times 10^{-8}$	$1.096\,31 \times 10^{-7}$	$3.456\,57 \times 10^{-7}$	$1.891\,03 \times 10^{-8}$	$2.883\,39 \times 10^{-5}$	$1.451\,33 \times 10^{-7}$	$2.006\,26 \times 10^{-8}$	$2.018\,98 \times 10^{-8}$
	0.00 %	$2.081\,62 \times 10^{-8}$	$1.681\,63 \times 10^{-7}$	1.6792×10^{-7}	$2.005\,59 \times 10^{-8}$	$2.972\,61 \times 10^{-5}$	$2.433\,26 \times 10^{-7}$	$2.204\,73 \times 10^{-8}$	$2.186\,64 \times 10^{-8}$
	6.00 %	2.1784×10^{-8}	$1.614\,53 \times 10^{-7}$	$3.331\,33 \times 10^{-7}$	$2.330\,51 \times 10^{-8}$	$3.198\,29 \times 10^{-5}$	$1.124\,08 \times 10^{-7}$	$2.437\,15 \times 10^{-8}$	$2.380\,49 \times 10^{-8}$
	12.00 %	$2.321\,73 \times 10^{-8}$	$2.443\,33 \times 10^{-7}$	$4.497\,66 \times 10^{-7}$	$2.701\,88 \times 10^{-8}$	$3.425\,77 \times 10^{-5}$	$3.270\,47 \times 10^{-7}$	$2.887\,29 \times 10^{-8}$	$2.773\,87 \times 10^{-8}$
	18.00 %	$2.452\,19 \times 10^{-8}$	$2.755\,54 \times 10^{-7}$	$2.021\,95 \times 10^{-7}$	$3.091\,43 \times 10^{-8}$	$3.651\,42 \times 10^{-5}$	$2.810\,88 \times 10^{-7}$	$3.097\,29 \times 10^{-8}$	3.2272×10^{-8}
ACCQ	-18.00 %	1.6616×10^{-8}	$2.882\,94 \times 10^{-7}$	$1.680\,67 \times 10^{-7}$	$1.573\,99 \times 10^{-8}$	$2.364\,74 \times 10^{-5}$	$2.257\,51 \times 10^{-7}$	$1.711\,77 \times 10^{-8}$	$1.727\,27 \times 10^{-8}$
	-12.00 %	$1.808\,86 \times 10^{-8}$	$2.448\,03 \times 10^{-7}$	$3.518\,38 \times 10^{-7}$	$1.917\,81 \times 10^{-8}$	$2.570\,06 \times 10^{-5}$	$1.334\,38 \times 10^{-7}$	$1.859\,17 \times 10^{-8}$	$1.884\,58 \times 10^{-8}$
	-6.00 %	$1.960\,97 \times 10^{-8}$	$2.423\,48 \times 10^{-7}$	$4.635\,87 \times 10^{-7}$	$2.169\,13 \times 10^{-8}$	$2.908\,28 \times 10^{-5}$	2.3688×10^{-7}	$2.010\,96 \times 10^{-8}$	$2.047\,32 \times 10^{-8}$
	0.00 %	$2.056\,92 \times 10^{-8}$	$2.444\,43 \times 10^{-7}$	$2.690\,63 \times 10^{-7}$	$2.680\,28 \times 10^{-8}$	$3.001\,17 \times 10^{-5}$	$1.925\,68 \times 10^{-7}$	$2.129\,68 \times 10^{-8}$	$2.187\,49 \times 10^{-8}$
	6.00 %	$2.204\,54 \times 10^{-8}$	$2.694\,11 \times 10^{-7}$	$3.517\,18 \times 10^{-7}$	$2.346\,81 \times 10^{-8}$	$3.231\,83 \times 10^{-5}$	$1.708\,18 \times 10^{-7}$	$2.446\,79 \times 10^{-8}$	$2.407\,65 \times 10^{-8}$
	12.00 %	$2.344\,17 \times 10^{-8}$	$8.578\,08 \times 10^{-8}$	$3.516\,82 \times 10^{-7}$	2.7193×10^{-8}	$3.467\,81 \times 10^{-5}$	$1.384\,12 \times 10^{-7}$	$2.994\,36 \times 10^{-8}$	$3.175\,25 \times 10^{-8}$
	18.00 %	$2.483\,94 \times 10^{-8}$	2.5094×10^{-7}	$8.203\,78 \times 10^{-10}$	$3.350\,82 \times 10^{-8}$	$3.691\,88 \times 10^{-5}$	$4.476\,52 \times 10^{-7}$	$3.184\,59 \times 10^{-8}$	$3.692\,96 \times 10^{-8}$
APC3	-18.00 %	$1.629\,56 \times 10^{-8}$	$1.649\,09 \times 10^{-7}$	$1.649\,09 \times 10^{-7}$	$1.458\,09 \times 10^{-8}$	$2.351\,06 \times 10^{-5}$	$1.963\,02 \times 10^{-7}$	$1.712\,37 \times 10^{-8}$	$1.912\,25 \times 10^{-8}$
	-12.00 %	$1.767\,56 \times 10^{-8}$	$1.684\,06 \times 10^{-7}$	$2.695\,36 \times 10^{-7}$	$1.879\,91 \times 10^{-8}$	$2.568\,27 \times 10^{-5}$	$1.182\,64 \times 10^{-7}$	$1.858\,58 \times 10^{-8}$	2.1578×10^{-8}
	-6.00 %	$1.915\,22 \times 10^{-8}$	$1.649\,09 \times 10^{-7}$	2.446×10^{-7}	$2.269\,37 \times 10^{-8}$	$2.909\,41 \times 10^{-5}$	$2.007\,41 \times 10^{-7}$	$2.010\,02 \times 10^{-8}$	$2.662\,01 \times 10^{-8}$
	0.00 %	$2.061\,01 \times 10^{-8}$	$2.422\,06 \times 10^{-7}$	$2.963\,13 \times 10^{-7}$	$2.594\,54 \times 10^{-8}$	$3.012\,95 \times 10^{-5}$	$3.711\,87 \times 10^{-7}$	$2.157\,37 \times 10^{-8}$	$3.512\,57 \times 10^{-8}$
	6.00 %	$2.209\,21 \times 10^{-8}$	$2.607\,44 \times 10^{-7}$	$2.562\,35 \times 10^{-7}$	$2.627\,68 \times 10^{-8}$	$3.230\,28 \times 10^{-5}$	$1.601\,03 \times 10^{-7}$	$2.337\,59 \times 10^{-8}$	$6.207\,92 \times 10^{-8}$
	12.00 %	$2.350\,17 \times 10^{-8}$	$2.373\,45 \times 10^{-7}$	$1.880\,26 \times 10^{-7}$	$3.017\,73 \times 10^{-8}$	$3.465\,99 \times 10^{-5}$	$8.109\,05 \times 10^{-7}$	$3.013\,04 \times 10^{-8}$	$9.047\,46 \times 10^{-8}$
	18.00 %	2.4873×10^{-8}	$1.990\,65 \times 10^{-7}$	$1.448\,42 \times 10^{-7}$	$3.225\,65 \times 10^{-8}$	$3.698\,38 \times 10^{-5}$	$1.412\,47 \times 10^{-7}$	$2.935\,75 \times 10^{-8}$	$1.895\,93 \times 10^{-7}$

Table A.42: The RMSE for the XZ-Direction fitting functions at a maximum field of 0.01.

Basis Set	Bond Length (%)	RHF Energy	RHF X Dipole	RHF Z Dipole	MP2 Energy	MP2 X Dipole	MP2 Z Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.195\,11 \times 10^{-8}$	$2.754\,01 \times 10^{-7}$	$1.892\,24 \times 10^{-7}$	$1.172\,34 \times 10^{-8}$	$1.815\,65 \times 10^{-5}$	$2.192\,08 \times 10^{-7}$	$1.273\,06 \times 10^{-8}$	1.3213×10^{-8}
	-12.00 %	$1.301\,07 \times 10^{-8}$	$2.092\,38 \times 10^{-7}$	$3.776\,39 \times 10^{-7}$	1.419×10^{-8}	$1.966\,99 \times 10^{-5}$	$2.023\,11 \times 10^{-7}$	$1.366\,41 \times 10^{-8}$	$1.383\,23 \times 10^{-8}$
	-6.00 %	$1.406\,43 \times 10^{-8}$	$1.673\,23 \times 10^{-7}$	$4.662\,46 \times 10^{-7}$	$1.405\,85 \times 10^{-8}$	$2.137\,83 \times 10^{-5}$	$1.593\,16 \times 10^{-7}$	$1.491\,69 \times 10^{-8}$	$1.499\,71 \times 10^{-8}$
	0.00 %	$1.512\,36 \times 10^{-8}$	$1.318\,71 \times 10^{-7}$	3.4764×10^{-7}	$1.631\,04 \times 10^{-8}$	$2.307\,27 \times 10^{-5}$	$1.546\,43 \times 10^{-7}$	$1.603\,06 \times 10^{-8}$	$1.621\,25 \times 10^{-8}$
	6.00 %	$1.619\,16 \times 10^{-8}$	$2.622\,64 \times 10^{-7}$	$3.642\,96 \times 10^{-7}$	$1.729\,71 \times 10^{-8}$	$2.484\,18 \times 10^{-5}$	$1.344\,53 \times 10^{-7}$	$1.834\,28 \times 10^{-8}$	$1.771\,59 \times 10^{-8}$
	12.00 %	$1.726\,17 \times 10^{-8}$	$2.913\,73 \times 10^{-7}$	$4.650\,82 \times 10^{-7}$	$2.051\,57 \times 10^{-8}$	$2.659\,01 \times 10^{-5}$	$2.287\,36 \times 10^{-7}$	$2.273\,47 \times 10^{-8}$	$2.108\,89 \times 10^{-8}$
	18.00 %	1.8244×10^{-8}	3.2833×10^{-7}	4.5813×10^{-7}	$4.931\,35 \times 10^{-8}$	2.8331×10^{-5}	$9.126\,87 \times 10^{-7}$	$2.329\,93 \times 10^{-8}$	$2.446\,71 \times 10^{-8}$
ACCQ	-18.00 %	$1.206\,18 \times 10^{-8}$	$2.478\,86 \times 10^{-7}$	$2.530\,32 \times 10^{-7}$	$1.146\,52 \times 10^{-8}$	$1.833\,86 \times 10^{-5}$	$1.845\,69 \times 10^{-7}$	$1.273\,01 \times 10^{-8}$	$1.283\,61 \times 10^{-8}$
	-12.00 %	$1.312\,21 \times 10^{-8}$	$1.971\,55 \times 10^{-7}$	$3.550\,94 \times 10^{-7}$	$1.393\,37 \times 10^{-8}$	$1.995\,27 \times 10^{-5}$	$1.165\,33 \times 10^{-7}$	$1.381\,59 \times 10^{-8}$	$1.399\,94 \times 10^{-8}$
	-6.00 %	$1.421\,45 \times 10^{-8}$	$3.141\,09 \times 10^{-7}$	$8.604\,47 \times 10^{-7}$	$1.631\,57 \times 10^{-8}$	$2.155\,51 \times 10^{-5}$	$2.206\,33 \times 10^{-7}$	$1.494\,11 \times 10^{-8}$	$1.521\,64 \times 10^{-8}$
	0.00 %	1.5289×10^{-8}	$2.470\,23 \times 10^{-7}$	$3.175\,28 \times 10^{-7}$	$2.027\,59 \times 10^{-8}$	$2.329\,95 \times 10^{-5}$	2.3921×10^{-7}	$1.577\,78 \times 10^{-8}$	$1.622\,83 \times 10^{-8}$
	6.00 %	$1.638\,26 \times 10^{-8}$	3.2929×10^{-7}	$3.224\,98 \times 10^{-7}$	$1.741\,89 \times 10^{-8}$	$2.508\,63 \times 10^{-5}$	$1.895\,99 \times 10^{-7}$	$1.840\,06 \times 10^{-8}$	1.7931×10^{-8}
	12.00 %	1.7463×10^{-8}	$2.819\,38 \times 10^{-7}$	$4.850\,72 \times 10^{-7}$	$2.064\,24 \times 10^{-8}$	$2.689\,98 \times 10^{-5}$	$1.716\,82 \times 10^{-7}$	$2.333\,13 \times 10^{-8}$	2.5013×10^{-8}
	18.00 %	$1.849\,53 \times 10^{-8}$	$2.816\,99 \times 10^{-7}$	$2.945\,73 \times 10^{-7}$	5.029×10^{-8}	$2.865\,67 \times 10^{-5}$	$8.904\,21 \times 10^{-7}$	$2.391\,65 \times 10^{-8}$	$2.817\,44 \times 10^{-8}$
APC3	-18.00 %	$1.211\,33 \times 10^{-8}$	$2.575\,52 \times 10^{-7}$	$3.050\,26 \times 10^{-7}$	$1.083\,76 \times 10^{-8}$	$1.823\,28 \times 10^{-5}$	$2.969\,48 \times 10^{-7}$	$1.271\,86 \times 10^{-8}$	$2.730\,47 \times 10^{-8}$
	-12.00 %	$1.313\,52 \times 10^{-8}$	$2.706\,55 \times 10^{-7}$	$2.455\,63 \times 10^{-7}$	$1.417\,62 \times 10^{-8}$	1.993×10^{-5}	$1.310\,06 \times 10^{-7}$	$1.381\,12 \times 10^{-8}$	$4.479\,77 \times 10^{-8}$
	-6.00 %	$1.423\,41 \times 10^{-8}$	$2.560\,93 \times 10^{-7}$	$4.962\,26 \times 10^{-7}$	$1.721\,84 \times 10^{-8}$	$2.156\,64 \times 10^{-5}$	1.5515×10^{-7}	$1.493\,38 \times 10^{-8}$	$6.728\,87 \times 10^{-8}$
	0.00 %	$1.531\,85 \times 10^{-8}$	$3.500\,51 \times 10^{-7}$	$2.743\,74 \times 10^{-7}$	$1.976\,09 \times 10^{-8}$	2.3383×10^{-5}	$3.025\,85 \times 10^{-7}$	$1.601\,79 \times 10^{-8}$	$1.101\,73 \times 10^{-7}$
	6.00 %	$1.641\,72 \times 10^{-8}$	$2.264\,77 \times 10^{-7}$	$4.450\,19 \times 10^{-7}$	1.9748×10^{-8}	$2.507\,35 \times 10^{-5}$	$1.847\,38 \times 10^{-7}$	$1.743\,88 \times 10^{-8}$	$2.127\,82 \times 10^{-7}$
	12.00 %	1.7485×10^{-8}	$2.616\,21 \times 10^{-7}$	$2.390\,36 \times 10^{-7}$	$2.272\,38 \times 10^{-8}$	$2.689\,92 \times 10^{-5}$	$6.133\,47 \times 10^{-7}$	$2.408\,25 \times 10^{-8}$	$3.865\,37 \times 10^{-7}$
	18.00 %	$1.849\,84 \times 10^{-8}$	$2.951\,04 \times 10^{-7}$	$2.039\,63 \times 10^{-7}$	$2.595\,98 \times 10^{-8}$	$2.868\,67 \times 10^{-5}$	$4.309\,57 \times 10^{-7}$	$2.193\,53 \times 10^{-8}$	$6.901\,52 \times 10^{-7}$

Table A.43: The RMSE for the XZ-Direction fitting functions at a maximum field of 0.015.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	1.1462×10^{-8}	1.1255×10^{-8}	1.2248×10^{-8}	1.2686×10^{-8}
	-12.00 %	$1.246\,81 \times 10^{-8}$	1.3639×10^{-8}	$1.311\,69 \times 10^{-8}$	$1.328\,35 \times 10^{-8}$
	-6.00 %	$1.347\,07 \times 10^{-8}$	$1.417\,19 \times 10^{-8}$	$1.429\,04 \times 10^{-8}$	$1.440\,72 \times 10^{-8}$
	0.00 %	$1.448\,68 \times 10^{-8}$	$1.565\,47 \times 10^{-8}$	$1.538\,34 \times 10^{-8}$	$1.556\,69 \times 10^{-8}$
	6.00 %	$1.554\,55 \times 10^{-8}$	$1.659\,18 \times 10^{-8}$	$1.761\,71 \times 10^{-8}$	$1.696\,38 \times 10^{-8}$
	12.00 %	$1.654\,94 \times 10^{-8}$	$1.974\,12 \times 10^{-8}$	$2.217\,21 \times 10^{-8}$	$2.029\,06 \times 10^{-8}$
	18.00 %	$1.749\,58 \times 10^{-8}$	5.4924×10^{-8}	$2.233\,48 \times 10^{-8}$	$2.354\,49 \times 10^{-8}$
ACCQ	-18.00 %	$1.155\,44 \times 10^{-8}$	$1.101\,94 \times 10^{-8}$	$1.218\,99 \times 10^{-8}$	$1.233\,82 \times 10^{-8}$
	-12.00 %	$1.259\,36 \times 10^{-8}$	$1.337\,64 \times 10^{-8}$	$1.322\,87 \times 10^{-8}$	$1.340\,51 \times 10^{-8}$
	-6.00 %	$1.365\,09 \times 10^{-8}$	$1.587\,14 \times 10^{-8}$	$1.436\,13 \times 10^{-8}$	$1.457\,19 \times 10^{-8}$
	0.00 %	$1.464\,02 \times 10^{-8}$	$1.955\,46 \times 10^{-8}$	$1.517\,28 \times 10^{-8}$	$1.554\,78 \times 10^{-8}$
	6.00 %	1.5706×10^{-8}	$1.675\,87 \times 10^{-8}$	$1.765\,35 \times 10^{-8}$	$1.721\,65 \times 10^{-8}$
	12.00 %	$1.672\,95 \times 10^{-8}$	$1.982\,46 \times 10^{-8}$	$2.248\,01 \times 10^{-8}$	$2.410\,72 \times 10^{-8}$
	18.00 %	1.7686×10^{-8}	$5.575\,51 \times 10^{-8}$	$2.290\,43 \times 10^{-8}$	$2.706\,41 \times 10^{-8}$
APC3	-18.00 %	1.168×10^{-8}	$1.042\,05 \times 10^{-8}$	$1.218\,31 \times 10^{-8}$	$3.742\,33 \times 10^{-8}$
	-12.00 %	$1.257\,58 \times 10^{-8}$	$1.360\,32 \times 10^{-8}$	$1.322\,35 \times 10^{-8}$	$7.086\,61 \times 10^{-8}$
	-6.00 %	$1.362\,93 \times 10^{-8}$	$1.652\,53 \times 10^{-8}$	$1.430\,11 \times 10^{-8}$	1.0893×10^{-7}
	0.00 %	$1.472\,87 \times 10^{-8}$	$1.895\,91 \times 10^{-8}$	$1.534\,08 \times 10^{-8}$	1.83×10^{-7}
	6.00 %	$1.577\,81 \times 10^{-8}$	$1.894\,56 \times 10^{-8}$	$1.673\,89 \times 10^{-8}$	$3.534\,58 \times 10^{-7}$
	12.00 %	$1.677\,24 \times 10^{-8}$	$2.174\,92 \times 10^{-8}$	$2.323\,89 \times 10^{-8}$	$6.445\,93 \times 10^{-7}$
	18.00 %	$1.773\,33 \times 10^{-8}$	$2.604\,34 \times 10^{-8}$	$2.100\,73 \times 10^{-8}$	$1.125\,14 \times 10^{-6}$

Table A.44: The RMSE for the XZ-Direction fitting functions at a maximum field of 0.02.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	$1.103\,44 \times 10^{-8}$	$1.082\,88 \times 10^{-8}$	$1.181\,58 \times 10^{-8}$	$1.224\,93 \times 10^{-8}$
	-12.00 %	$1.201\,19 \times 10^{-8}$	$1.311\,32 \times 10^{-8}$	$1.269\,27 \times 10^{-8}$	$1.286\,16 \times 10^{-8}$
	-6.00 %	$1.301\,66 \times 10^{-8}$	1.362×10^{-8}	$1.386\,49 \times 10^{-8}$	1.4007×10^{-8}
	0.00 %	$1.174\,47 \times 10^{-6}$	$1.710\,08 \times 10^{-6}$	1.6035×10^{-6}	$1.728\,56 \times 10^{-6}$
	6.00 %	$1.500\,89 \times 10^{-8}$	1.6318×10^{-8}	$1.696\,41 \times 10^{-8}$	$1.659\,27 \times 10^{-8}$
	12.00 %	$1.600\,67 \times 10^{-8}$	$1.901\,22 \times 10^{-8}$	$2.134\,96 \times 10^{-8}$	$1.983\,86 \times 10^{-8}$
	18.00 %	$1.686\,74 \times 10^{-8}$	$5.604\,85 \times 10^{-8}$	$2.158\,46 \times 10^{-8}$	$2.268\,89 \times 10^{-8}$
ACCQ	-18.00 %	$1.118\,31 \times 10^{-8}$	$1.108\,47 \times 10^{-8}$	$1.184\,31 \times 10^{-8}$	$1.205\,82 \times 10^{-8}$
	-12.00 %	$1.216\,75 \times 10^{-8}$	$1.300\,03 \times 10^{-8}$	$1.286\,37 \times 10^{-8}$	$1.308\,21 \times 10^{-8}$
	-6.00 %	1.3241×10^{-8}	1.5265×10^{-8}	$1.403\,03 \times 10^{-8}$	$1.423\,45 \times 10^{-8}$
	0.00 %	$1.412\,16 \times 10^{-6}$	$2.072\,01 \times 10^{-6}$	$1.900\,79 \times 10^{-6}$	2.0626×10^{-6}
	6.00 %	$1.522\,62 \times 10^{-8}$	$1.683\,28 \times 10^{-8}$	$1.712\,46 \times 10^{-8}$	$1.698\,79 \times 10^{-8}$
	12.00 %	$1.622\,46 \times 10^{-8}$	$1.903\,14 \times 10^{-8}$	$2.188\,56 \times 10^{-8}$	$2.337\,93 \times 10^{-8}$
	18.00 %	$1.719\,24 \times 10^{-8}$	$5.644\,43 \times 10^{-8}$	$2.240\,12 \times 10^{-8}$	2.6254×10^{-8}
APC3	-18.00 %	$1.141\,15 \times 10^{-8}$	$1.060\,23 \times 10^{-8}$	$1.204\,75 \times 10^{-8}$	$4.948\,99 \times 10^{-8}$
	-12.00 %	$1.228\,64 \times 10^{-8}$	$1.378\,65 \times 10^{-8}$	$1.315\,37 \times 10^{-8}$	$1.153\,21 \times 10^{-7}$
	-6.00 %	$1.331\,79 \times 10^{-8}$	$1.621\,63 \times 10^{-8}$	$1.424\,38 \times 10^{-8}$	$1.741\,75 \times 10^{-7}$
	0.00 %	$1.680\,19 \times 10^{-6}$	$2.549\,28 \times 10^{-6}$	$2.289\,41 \times 10^{-6}$	$2.774\,32 \times 10^{-6}$
	6.00 %	$1.538\,53 \times 10^{-8}$	$1.941\,57 \times 10^{-8}$	$1.673\,19 \times 10^{-8}$	$5.801\,77 \times 10^{-7}$
	12.00 %	$1.642\,75 \times 10^{-8}$	$2.207\,72 \times 10^{-8}$	$2.301\,93 \times 10^{-8}$	$1.083\,05 \times 10^{-6}$
	18.00 %	$1.742\,62 \times 10^{-8}$	$2.926\,54 \times 10^{-8}$	$2.170\,78 \times 10^{-8}$	1.8892×10^{-6}

A.7 Polarizabilities and Hyperpolarizabilities at Higher Fields

α_{xx} Values

Table A.45: The α_{xx} values for a CO_2 molecule at a maximum field of 0.005 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	9.3407	9.3409	10.0436	10.0440	9.8748	9.9962
	-12.00 %	10.1475	10.1475	10.9235	10.9241	10.7220	10.8621
	-6.00 %	10.9740	10.9741	11.8414	11.8420	11.5959	11.7575
	0.00 %	11.8073	11.8071	12.7852	12.7861	12.4822	12.6673
	6.00 %	12.6343	12.6344	13.7438	13.7450	13.3662	13.5762
	12.00 %	13.4413	13.4412	14.7069	14.7079	14.2335	14.4687
	18.00 %	14.2124	14.2125	15.6664	15.6678	15.0698	15.3311
ACCQ	-18.00 %	9.4240	9.4238	10.1272	10.1280	9.9314	10.0604
	-12.00 %	10.2451	10.2450	11.0222	11.0231	10.7905	10.9385
	-6.00 %	11.0880	11.0879	11.9579	11.9590	11.6786	11.8486
	0.00 %	11.9387	11.9387	12.9219	12.9230	12.5806	12.7748
	6.00 %	12.7836	12.7836	13.9030	13.9039	13.4815	13.7009
	12.00 %	13.6086	13.6087	14.8907	14.8918	14.3669	14.6119
	18.00 %	14.3984	14.3984	15.8783	15.8796	15.2230	15.4945
APC3	-18.00 %	9.4340	9.4341	10.1179	10.1241	9.9201	10.0410
	-12.00 %	10.2558	10.2558	11.0203	11.0196	10.7846	10.9294
	-6.00 %	11.1003	11.1002	11.9575	11.9584	11.6733	11.8409
	0.00 %	11.9536	11.9536	12.9269	12.9277	12.5789	12.7715
	6.00 %	12.8018	12.8020	13.9154	13.9168	13.4843	13.7026
	12.00 %	13.6309	13.6307	14.9142	14.9152	14.3771	14.6220
	18.00 %	14.4253	14.4252	15.9153	15.9163	15.2419	15.5141

Table A.46: The α_{xx} values for a CO_2 molecule at a maximum field of 0.01 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	9.3408	9.3407	10.0435	10.0442	9.8748	9.9963
	-12.00 %	10.1475	10.1475	10.9236	10.9244	10.7219	10.8621
	-6.00 %	10.9740	10.9740	11.8413	11.8422	11.5958	11.7573
	0.00 %	11.8073	11.8073	12.7852	12.7862	12.4822	12.6673
	6.00 %	12.6343	12.6344	13.7438	13.7449	13.3662	13.5762
	12.00 %	13.4412	13.4412	14.7068	14.7080	14.2335	14.4687
	18.00 %	14.2124	14.2125	15.6664	15.6677	15.0690	15.3302
ACCQ	-18.00 %	9.4239	9.4239	10.1272	10.1280	9.9314	10.0604
	-12.00 %	10.2451	10.2451	11.0222	11.0231	10.7905	10.9385
	-6.00 %	11.0880	11.0879	11.9578	11.9588	11.6786	11.8485
	0.00 %	11.9387	11.9387	12.9220	12.9229	12.5806	12.7747
	6.00 %	12.7836	12.7836	13.9030	13.9040	13.4815	13.7009
	12.00 %	13.6086	13.6086	14.8907	14.8918	14.3669	14.6119
	18.00 %	14.3984	14.3984	15.8783	15.8795	15.2223	15.4933
APC3	-18.00 %	9.4340	9.4340	10.1225	10.1241	9.9249	10.0525
	-12.00 %	10.2558	10.2558	11.0190	11.0196	10.7840	10.9303
	-6.00 %	11.1003	11.1004	11.9575	11.9582	11.6735	11.8416
	0.00 %	11.9536	11.9536	12.9268	12.9277	12.5787	12.7714
	6.00 %	12.8018	12.8018	13.9156	13.9167	13.4847	13.7031
	12.00 %	13.6308	13.6308	14.9141	14.9151	14.3770	14.6218
	18.00 %	14.4253	14.4253	15.9151	15.9163	15.2418	15.5141

Table A.47: The α_{xx} values for a CO_2 molecule at a maximum field of 0.015 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	9.3408	10.0435	9.8748	9.9964
	-12.00 %	10.1475	10.9236	10.7219	10.8621
	-6.00 %	10.9740	11.8413	11.5959	11.7575
	0.00 %	11.8073	12.7852	12.4822	12.6673
	6.00 %	12.6343	13.7438	13.3662	13.5761
	12.00 %	13.4412	14.7068	14.2334	14.4688
	18.00 %	14.2124	15.6664	15.0691	15.3303
ACCQ	-18.00 %	9.4239	10.1272	9.9314	10.0604
	-12.00 %	10.2451	11.0222	10.7905	10.9385
	-6.00 %	11.0879	11.9578	11.6786	11.8486
	0.00 %	11.9387	12.9219	12.5806	12.7747
	6.00 %	12.7836	13.9030	13.4815	13.7008
	12.00 %	13.6086	14.8907	14.3668	14.6118
	18.00 %	14.3984	15.8782	15.2226	15.4938
APC3	-18.00 %	9.4340	10.1232	9.9253	10.0523
	-12.00 %	10.2558	11.0188	10.7839	10.9302
	-6.00 %	11.1003	11.9574	11.6734	11.8416
	0.00 %	11.9536	12.9268	12.5788	12.7714
	6.00 %	12.8018	13.9156	13.4847	13.7031
	12.00 %	13.6308	14.9140	14.3769	14.6218
	18.00 %	14.4252	15.9150	15.2417	15.5140

Table A.48: The α_{xx} values for a CO_2 molecule at a maximum field of 0.02 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	9.3407	10.0435	9.8748	9.9964
	-12.00 %	10.1475	10.9235	10.7219	10.8620
	-6.00 %	10.9740	11.8413	11.5959	11.7576
	0.00 %	11.8072	12.7851	12.4822	12.6672
	6.00 %	12.6343	13.7438	13.3661	13.5761
	12.00 %	13.4411	14.7068	14.2334	14.4687
	18.00 %	14.2123	15.6663	15.0693	15.3305
ACCQ	-18.00 %	9.4239	10.1272	9.9314	10.0604
	-12.00 %	10.2450	11.0221	10.7905	10.9385
	-6.00 %	11.0879	11.9578	11.6786	11.8486
	0.00 %	11.9386	12.9219	12.5805	12.7746
	6.00 %	12.7836	13.9029	13.4814	13.7007
	12.00 %	13.6085	14.8906	14.3667	14.6117
	18.00 %	14.3983	15.8781	15.2227	15.4940
APC3	-18.00 %	9.4340	10.1232	9.9252	10.0522
	-12.00 %	10.2557	11.0187	10.7838	10.9301
	-6.00 %	11.1002	11.9573	11.6734	11.8415
	0.00 %	11.9535	12.9266	12.5786	12.7713
	6.00 %	12.8017	13.9154	13.4846	13.7029
	12.00 %	13.6306	14.9138	14.3768	14.6215
	18.00 %	14.4251	15.9147	15.2415	15.5137

α_{zz} Values

Table A.49: The α_{zz} values for a CO_2 molecule at a maximum field of 0.005 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	16.4810	16.4809	18.1105	18.1111	17.8219	17.9981
	-12.00 %	18.6227	18.6228	20.7050	20.7067	20.2984	20.5077
	-6.00 %	21.0229	21.0233	23.7745	23.7775	23.1531	23.4071
	0.00 %	23.6553	23.6554	27.3718	27.3765	26.3800	26.6954
	6.00 %	26.4840	26.4841	31.5501	31.5516	29.9535	30.3625
	12.00 %	29.4704	29.4706	36.2955	36.3006	33.8362	34.3997
	18.00 %	32.5922	32.5917	41.4157	41.4492	37.9841	38.8170
ACCQ	-18.00 %	16.4857	16.4855	18.0974	18.0980	17.7670	17.9525
	-12.00 %	18.6257	18.6257	20.6891	20.6908	20.2346	20.4548
	-6.00 %	21.0221	21.0225	23.7515	23.7556	23.0755	23.3423
	0.00 %	23.6508	23.6510	27.3442	27.3467	26.2860	26.6174
	6.00 %	26.4784	26.4785	31.5145	31.5152	29.8433	30.2721
	12.00 %	29.4675	29.4679	36.2561	36.2612	33.7148	34.2985
	18.00 %	32.5963	32.5962	41.3767	41.4106	37.8508	38.7111
APC3	-18.00 %	16.4849	16.4850	18.0913	18.0919	17.7588	17.9441
	-12.00 %	18.6236	18.6235	20.6812	20.6828	20.2238	20.4434
	-6.00 %	21.0184	21.0185	23.7444	23.7454	23.0619	23.3285
	0.00 %	23.6451	23.6453	27.3304	27.3346	26.2693	26.6002
	6.00 %	26.4702	26.4702	31.4987	31.5015	29.8260	30.2535
	12.00 %	29.4572	29.4571	36.2431	36.2462	33.6947	34.2786
	18.00 %	32.5846	32.5843	41.3835	41.3969	37.8318	38.6926

Table A.50: The α_{zz} values for a CO_2 molecule at a maximum field of 0.01 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	16.4810	16.4807	18.1100	18.1113	17.8220	17.9985
	-12.00 %	18.6226	18.6225	20.7050	20.7066	20.2983	20.5076
	-6.00 %	21.0229	21.0229	23.7757	23.7774	23.1531	23.4071
	0.00 %	23.6554	23.6553	27.3747	27.3764	26.3793	26.6950
	6.00 %	26.4841	26.4840	31.5493	31.5514	29.9546	30.3627
	12.00 %	29.4704	29.4704	36.2965	36.3004	33.8410	34.4020
	18.00 %	32.5920	32.5922	41.4413	41.4503	37.9851	38.8196
ACCQ	-18.00 %	16.4856	16.4854	18.0965	18.0977	17.7669	17.9525
	-12.00 %	18.6257	18.6256	20.6890	20.6908	20.2346	20.4546
	-6.00 %	21.0221	21.0220	23.7531	23.7554	23.0754	23.3423
	0.00 %	23.6509	23.6507	27.3451	27.3466	26.2854	26.6171
	6.00 %	26.4784	26.4783	31.5133	31.5152	29.8445	30.2724
	12.00 %	29.4676	29.4675	36.2572	36.2612	33.7174	34.3021
	18.00 %	32.5964	32.5965	41.4027	41.4116	37.8511	38.7136
APC3	-18.00 %	16.4850	16.4848	18.0908	18.0920	17.7588	17.9441
	-12.00 %	18.6236	18.6236	20.6820	20.6828	20.2237	20.4434
	-6.00 %	21.0185	21.0184	23.7440	23.7453	23.0617	23.3283
	0.00 %	23.6452	23.6451	27.3321	27.3345	26.2692	26.6001
	6.00 %	26.4703	26.4702	31.4990	31.5013	29.8264	30.2534
	12.00 %	29.4572	29.4571	36.2432	36.2461	33.6980	34.2816
	18.00 %	32.5847	32.5848	41.3891	41.3973	37.8320	38.6933

Table A.51: The α_{zz} values for a CO_2 molecule at a maximum field of 0.015 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	16.4809	18.1099	17.8220	17.9985
	-12.00 %	18.6226	20.7049	20.2984	20.5077
	-6.00 %	21.0229	23.7758	23.1530	23.4070
	0.00 %	23.6552	27.3746	26.3792	26.6949
	6.00 %	26.4839	31.5493	29.9547	30.3626
	12.00 %	29.4704	36.2970	33.8413	34.4020
	18.00 %	32.5920	41.4442	37.9853	38.8198
ACCQ	-18.00 %	16.4856	18.0964	17.7669	17.9525
	-12.00 %	18.6257	20.6892	20.2347	20.4547
	-6.00 %	21.0222	23.7534	23.0754	23.3424
	0.00 %	23.6508	27.3449	26.2852	26.6169
	6.00 %	26.4783	31.5131	29.8447	30.2724
	12.00 %	29.4676	36.2577	33.7173	34.3021
	18.00 %	32.5963	41.4056	37.8512	38.7138
APC3	-18.00 %	16.4850	18.0908	17.7587	17.9440
	-12.00 %	18.6235	20.6817	20.2235	20.4433
	-6.00 %	21.0184	23.7437	23.0617	23.3282
	0.00 %	23.6451	27.3323	26.2690	26.6002
	6.00 %	26.4702	31.4989	29.8264	30.2533
	12.00 %	29.4571	36.2431	33.6979	34.2816
	18.00 %	32.5845	41.3927	37.8318	38.6935

Table A.52: The α_{zz} values for a CO_2 molecule at a maximum field of 0.02 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	16.4809	18.1098	17.8219	17.9984
	-12.00 %	18.6225	20.7049	20.2983	20.5076
	-6.00 %	21.0228	23.7757	23.1528	23.4068
	0.00 %	23.6552	27.3744	26.3790	26.6947
	6.00 %	26.4839	31.5491	29.9546	30.3625
	12.00 %	29.4703	36.2973	33.8410	34.4017
	18.00 %	32.5920	41.4452	37.9853	38.8197
ACCQ	-18.00 %	16.4855	18.0963	17.7668	17.9524
	-12.00 %	18.6256	20.6890	20.2345	20.4546
	-6.00 %	21.0221	23.7534	23.0753	23.3422
	0.00 %	23.6507	27.3447	26.2851	26.6167
	6.00 %	26.4783	31.5129	29.8446	30.2722
	12.00 %	29.4674	36.2576	33.7171	34.3018
	18.00 %	32.5962	41.4066	37.8510	38.7137
APC3	-18.00 %	16.4849	18.0906	17.7586	17.9438
	-12.00 %	18.6235	20.6814	20.2234	20.4430
	-6.00 %	21.0183	23.7435	23.0615	23.3280
	0.00 %	23.6450	27.3321	26.2687	26.5998
	6.00 %	26.4701	31.4986	29.8262	30.2530
	12.00 %	29.4570	36.2429	33.6975	34.2812
	18.00 %	32.5843	41.3930	37.8314	38.6931

γ_{xxxx} Values

Table A.53: The γ_{xxxx} values for a CO_2 molecule at a maximum field of 0.005 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
	-18.00 %	346.9412	270.3963	370.1795	473.1935	389.3296	501.2666
	-12.00 %	371.0108	375.2914	534.2168	603.7296	423.2383	478.3901
	-6.00 %	453.0588	403.2634	563.3234	673.6597	529.0821	589.4860
ACCT	0.00 %	516.0155	603.7296	748.4278	748.2517	683.9845	713.9616
	6.00 %	677.0502	624.7086	908.0542	874.1259	836.7157	866.7319
	12.00 %	689.4714	734.2657	1035.2291	1072.2611	948.1637	1031.0431
	18.00 %	858.1936	848.4848	1259.8758	1200.4662	1087.5251	1220.5682
	-18.00 %	365.2599	382.2844	551.0978	473.1935	496.1025	489.2464
	-12.00 %	412.7243	473.1935	581.0357	603.7296	565.7587	602.5527
	-6.00 %	503.4085	543.1235	717.1206	673.6597	664.0618	700.8558
ACCQ	0.00 %	648.2958	652.6807	873.5879	874.1259	782.6691	831.0431
	6.00 %	745.9925	778.5548	1075.5636	1074.5921	980.4587	983.8525
	12.00 %	870.4289	853.1469	1283.8672	1256.4103	1110.2646	1220.5291
	18.00 %	986.2878	993.0070	1486.5372	1452.2144	1301.7262	1412.4505
	-18.00 %	453.0588	403.2634	3037.8796	603.7296	3186.6399	5966.6389
	-12.00 %	512.9737	526.8065	-163.2843	722.6107	249.6259	1267.2796
	-6.00 %	661.8514	678.3217	935.6350	825.1748	908.6997	1222.1331
APC3	0.00 %	773.7200	778.5548	975.1968	1069.9301	883.4173	984.7425
	6.00 %	900.2494	874.1259	1391.4617	1256.4103	1339.8993	1501.2470
	12.00 %	991.6573	1069.9301	1484.8452	1517.4825	1323.3214	1396.3714
	18.00 %	1174.8252	1244.7552	1778.2972	1848.4848	1507.9075	1758.7951

Table A.54: The γ_{xxxx} values for a CO_2 molecule at a maximum field of 0.01 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
	-18.00 %	310.3763	310.5194	415.7607	415.3203	386.3863	424.0771
	-12.00 %	374.6687	375.6096	498.8428	499.7342	467.5857	492.6077
	-6.00 %	448.8258	450.9627	606.5003	606.5922	577.1822	636.5720
ACCT	0.00 %	537.3532	534.6832	731.0927	730.2083	668.0766	728.3939
	6.00 %	632.2288	631.0704	885.3137	879.7818	800.4447	873.6101
	12.00 %	733.4281	736.4723	1052.5842	1049.1875	940.0251	1056.8337
	18.00 %	839.6272	834.7318	1247.8339	1241.4766	1141.5809	1274.8214
	-18.00 %	378.5098	379.9320	503.7269	507.0615	459.0215	490.4894
	-12.00 %	449.0535	446.7559	599.4789	591.4754	547.7858	586.7341
	-6.00 %	535.8477	540.3463	723.0511	709.8213	667.9414	738.3313
ACCQ	0.00 %	633.9864	635.6471	869.6449	866.5141	787.4761	852.4898
	6.00 %	747.7442	753.5076	1040.5739	1045.4199	937.2494	1018.8963
	12.00 %	866.5754	868.1784	1245.0347	1246.1688	1099.2790	1209.5533
	18.00 %	989.2749	995.9550	1469.6562	1467.7438	1359.7019	1545.6341
	-18.00 %	444.6736	444.0053	718.0200	604.2115	608.9905	572.2682
	-12.00 %	532.0537	525.2525	700.4378	726.6949	642.2033	687.9279
	-6.00 %	639.9968	633.4512	851.8770	875.4594	781.0922	858.0588
APC3	0.00 %	760.9959	760.1877	1064.4464	1062.4552	958.9982	1039.3045
	6.00 %	900.4940	897.9497	1288.4458	1284.1920	1143.9630	1250.1155
	12.00 %	1047.0803	1049.7885	1537.5007	1537.6419	1348.4976	1479.3594
	18.00 %	1202.6391	1206.0421	1826.8740	1834.7318	1575.7127	1748.3220

Table A.55: The γ_{xxxx} values for a CO_2 molecule at a maximum field of 0.015 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
	-18.00 %	309.4568	416.8888	391.6966	415.5907
	-12.00 %	376.2870	496.5837	465.6375	494.2551
	-6.00 %	451.5794	607.2790	564.6633	608.2086
ACCT	0.00 %	535.3138	734.0057	676.4564	728.5379
	6.00 %	635.1497	887.1200	800.9782	878.5169
	12.00 %	738.5421	1059.0874	948.8512	1042.1185
	18.00 %	843.6606	1251.9054	1137.7516	1273.5520
	-18.00 %	378.7935	500.3758	462.6036	494.8138
	-12.00 %	448.5684	597.7587	548.7199	592.0483
	-6.00 %	538.9631	722.0075	662.1574	710.2081
ACCQ	0.00 %	636.3922	873.6380	787.2449	856.9769
	6.00 %	749.2595	1046.6051	937.9860	1027.7870
	12.00 %	870.0077	1249.9045	1104.4615	1219.6432
	18.00 %	997.5122	1477.9289	1306.8248	1462.0846
	-18.00 %	446.8792	614.1831	552.9942	594.8034
	-12.00 %	533.1527	728.3436	665.9074	700.2517
	-6.00 %	644.1489	880.1401	801.1953	863.6780
APC3	0.00 %	764.3895	1064.4983	957.8975	1043.9323
	6.00 %	906.4442	1289.6785	1147.3768	1251.1258
	12.00 %	1051.7093	1547.4645	1357.6808	1494.6908
	18.00 %	1208.9709	1843.8053	1588.1506	1767.6264

Table A.56: The γ_{xxxx} values for a CO_2 molecule at a maximum field of 0.02 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	314.5599	416.0311	389.6031	416.0706
	-12.00 %	375.5832	502.1429	467.6240	499.6109
	-6.00 %	452.7941	608.8146	561.1381	602.9360
	0.00 %	540.4417	739.2806	676.0735	735.4433
	6.00 %	638.2166	890.3292	809.1443	883.9765
	12.00 %	741.2593	1063.2603	951.8378	1048.8823
	18.00 %	849.2434	1260.1781	1121.7291	1252.2300
ACCQ	-18.00 %	378.9687	506.4586	465.6577	496.9508
	-12.00 %	453.1116	602.9102	553.2995	592.8312
	-6.00 %	541.1198	726.3449	660.7765	711.7541
	0.00 %	643.5425	875.9250	796.1977	861.5357
	6.00 %	755.5527	1054.0898	945.4665	1033.5769
	12.00 %	878.1413	1258.7676	1113.2717	1226.5782
	18.00 %	1003.9394	1491.6031	1298.5602	1451.3855
APC3	-18.00 %	448.4376	612.3652	559.1997	600.0599
	-12.00 %	537.6981	732.4576	667.6279	712.5004
	-6.00 %	646.5431	887.2518	802.3375	867.3123
	0.00 %	771.0291	1079.4803	968.1523	1050.6324
	6.00 %	910.0129	1304.6432	1158.8618	1266.4008
	12.00 %	1064.5342	1566.7255	1371.7901	1512.3091
	18.00 %	1223.4145	1865.4791	1605.6627	1789.3088

γ_{zzzz} Values

Table A.57: The γ_{zzzz} values for a CO_2 molecule at a maximum field of 0.005 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	571.1282	543.1235	582.9429	876.4569	854.2716	985.7597
	-12.00 %	604.8804	526.8065	821.2040	853.1469	803.9317	883.3390
	-6.00 %	641.5962	550.1165	1178.1114	904.4289	846.0267	906.6458
	0.00 %	676.7470	662.0047	2590.4836	920.7459	550.4621	783.9601
	6.00 %	748.2517	696.9697	616.2257	923.0769	1453.9782	1113.8246
	12.00 %	828.4219	759.9068	1538.9603	923.0769	3507.9661	2215.3552
	18.00 %	921.5903	1125.8741	14567.2256	1319.3473	1589.5447	2308.4454
ACCQ	-18.00 %	627.3852	648.0186	494.3714	874.1259	852.5307	957.9539
	-12.00 %	733.2681	652.6807	896.6306	1000.0000	957.2204	940.3883
	-6.00 %	740.0851	592.0746	1843.9532	995.3380	980.4489	1075.2506
	0.00 %	829.0088	729.6037	1687.1338	1069.9301	698.7432	888.1314
	6.00 %	828.4219	792.5408	565.8859	1151.5151	1683.5151	1294.5278
	12.00 %	992.8212	836.8298	1767.8908	1151.5152	2517.7563	3009.6435
	18.00 %	1163.0006	1207.4592	15065.4309	1564.1026	1371.1379	2529.8058
APC3	-18.00 %	755.2839	673.6597	806.2203	1074.5921	938.5985	1012.2255
	-12.00 %	775.7739	792.5408	1532.9649	1144.5221	897.3446	1052.3546
	-6.00 %	842.5840	792.5532	1003.0613	1156.1772	990.7379	1070.7712
	0.00 %	908.0933	843.8228	2170.7174	1251.7482	1071.8079	1255.4550
	6.00 %	989.6621	951.0489	1560.2719	1265.7343	1468.0718	1276.2678
	12.00 %	1082.8794	1076.9231	1431.3658	1351.9814	3077.5490	3051.6602
	18.00 %	1249.8998	1375.2914	4963.9102	1603.7296	1507.1446	1874.0183

Table A.58: The γ_{zzzz} values for a CO_2 molecule at a maximum field of 0.01 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole	MP2 Energy	MP2 Dipole	CCSD Energy	CCSD(T) Energy
	-18.00 %	574.7409	578.3695	835.1037	841.1576	783.6650	853.3306
	-12.00 %	612.4233	603.9341	894.9555	887.2246	851.2526	912.0155
	-6.00 %	661.5857	653.6070	958.3094	937.4754	854.6949	930.3224
ACCT	0.00 %	678.8267	695.1437	943.9564	959.1568	906.5426	953.3694
	6.00 %	736.7454	751.9821	964.7129	968.0790	966.9233	992.7321
	12.00 %	837.8275	822.4811	1094.7587	955.9901	1012.3120	986.9707
	18.00 %	978.5486	963.3405	1590.7730	974.6666	1093.2594	990.5048
	-18.00 %	646.3628	659.2700	931.1644	945.7966	865.3847	929.0005
	-12.00 %	691.4782	683.4940	1031.0702	1000.0000	931.9345	1002.0898
	-6.00 %	758.0449	749.7631	1120.1914	1055.0586	978.6781	1067.6441
ACCQ	0.00 %	784.2366	800.4762	1064.3688	1106.8581	1008.1351	1073.2470
	6.00 %	865.6638	864.9886	1108.9034	1139.5419	1121.5825	1157.4376
	12.00 %	964.5089	952.3611	1277.6903	1155.4446	1132.6881	1178.1511
	18.00 %	1111.0599	1103.9456	1851.9667	1237.8707	1235.8622	1204.2744
	-18.00 %	707.4182	719.9454	1039.1511	1041.9758	951.1414	1024.3603
	-12.00 %	756.5122	757.3446	1058.4238	1119.9639	1001.7897	1085.0837
	-6.00 %	808.9928	816.7718	1151.7873	1198.9922	1090.2032	1165.8101
APC3	0.00 %	867.6897	880.5677	1317.8013	1264.0131	1128.0760	1255.2692
	6.00 %	953.3109	958.3709	1313.0709	1320.5973	1242.9225	1316.3050
	12.00 %	1054.9955	1066.4078	1388.3823	1374.7082	1297.9695	1387.1391
	18.00 %	1212.7976	1227.6772	2156.8105	1478.1222	1414.1873	1457.7330

Table A.59: The γ_{zzzz} values for a CO_2 molecule at a maximum field of 0.015 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
	-18.00 %	582.1802	846.8340	789.8520	848.6385
	-12.00 %	613.6036	903.8194	835.2119	900.3130
	-6.00 %	654.8406	935.4291	878.2421	946.7731
ACCT	0.00 %	706.2626	954.4320	907.6765	985.5131
	6.00 %	761.5854	962.0651	957.9218	1007.0125
	12.00 %	838.9212	1011.6254	969.3923	990.9043
	18.00 %	975.6386	1125.1443	1047.3938	957.2731
	-18.00 %	648.0981	952.9286	867.3690	935.7024
	-12.00 %	690.5573	1009.3250	918.2295	995.2530
	-6.00 %	743.4750	1078.6117	978.8457	1054.2720
ACCQ	0.00 %	800.1595	1104.7463	1029.4671	1110.3569
	6.00 %	870.2615	1140.0621	1093.4263	1154.6311
	12.00 %	960.9364	1206.5399	1138.6712	1179.9937
	18.00 %	1114.9232	1383.5003	1229.2668	1177.2075
	-18.00 %	712.5135	1044.8861	958.0940	1031.6911
	-12.00 %	763.5999	1110.6990	1026.2838	1101.1585
	-6.00 %	820.6673	1195.2151	1090.1573	1186.2642
APC3	0.00 %	886.4253	1278.9902	1153.2298	1252.3962
	6.00 %	961.5326	1332.8593	1245.3415	1334.2844
	12.00 %	1072.5424	1408.1400	1318.6037	1382.0102
	18.00 %	1243.5673	1576.7183	1446.4968	1416.7382

Table A.60: The γ_{zzzz} values for a CO_2 molecule at a maximum field of 0.02 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	581.6545	852.6440	796.0334	854.4031
	-12.00 %	621.4777	901.6668	840.9615	904.3033
	-6.00 %	661.8166	945.7874	886.3553	955.3840
	0.00 %	709.0652	973.1020	923.8754	994.8320
	6.00 %	762.7542	980.3749	962.9116	1018.9509
	12.00 %	845.1175	989.8811	989.9593	1008.0385
	18.00 %	980.7988	1051.6736	1051.6442	966.9519
ACCQ	-18.00 %	656.0934	954.5238	876.7719	943.2228
	-12.00 %	698.1563	1020.4763	929.7288	1002.3368
	-6.00 %	746.5885	1079.2700	985.7363	1065.4849
	0.00 %	805.0951	1120.8773	1039.1319	1123.1601
	6.00 %	874.5946	1158.2836	1097.8422	1171.7750
	12.00 %	971.9591	1212.4957	1154.0308	1197.0200
	18.00 %	1124.1237	1305.8071	1240.9522	1184.5067
APC3	-18.00 %	719.4699	1059.5132	970.6078	1047.0140
	-12.00 %	770.5436	1132.7226	1037.1018	1121.3846
	-6.00 %	827.9539	1215.9167	1105.0464	1200.4434
	0.00 %	892.8222	1294.2116	1179.8324	1277.6850
	6.00 %	973.7887	1356.4313	1259.8949	1354.5353
	12.00 %	1085.0187	1424.8011	1346.4458	1416.5704
	18.00 %	1257.4491	1553.2534	1475.7910	1449.1904

γ_{xxzz} Values

Table A.61: The γ_{xxzz} values for a CO_2 molecule at a maximum field of 0.005 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole X	RHF Dipole Z	MP2 Energy	MP2 Dipole X	MP2 Dipole Z	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	-148.9410	151.6179	192.5734	687.9235	2072.9284	362.2648	642.8770	714.6949
	-12.00 %	-158.5652	255.1077	191.6041	-221.8106	2255.7791	389.2133	-200.4360	718.1596
	-6.00 %	-178.3523	239.1910	141.8952	-286.1914	2487.4015	413.4310	829.0997	817.6775
	0.00 %	-194.6991	244.8931	225.4733	1902.4030	2807.5753	445.9523	-201.6512	835.8189
	6.00 %	842.1724	354.3779	253.3779	910.2223	2967.8051	488.8184	1250.1565	1040.9797
	12.00 %	942.6668	313.4639	280.7494	1774.6486	3257.7863	443.3318	1575.5798	1390.8126
	18.00 %	1003.0902	402.8573	444.4613	1647.5002	3399.6576	659.7701	1738.1338	1835.8693
ACCQ	-18.00 %	-161.3635	193.4388	230.1321	-170.1841	2042.5757	477.4092	738.6681	676.1795
	-12.00 %	-186.9128	226.8691	235.1721	-242.1987	2220.3874	480.0498	719.3821	755.8597
	-6.00 %	-203.1523	322.2347	138.8976	1013.9078	2571.3745	461.1365	820.3543	858.6280
	0.00 %	788.4207	281.3207	269.2491	1542.0036	2797.0476	502.0028	825.0562	918.9751
	6.00 %	881.4597	285.5144	340.1961	946.9766	3020.3896	514.2995	1326.3035	1136.3403
	12.00 %	958.0294	350.7561	325.4344	1907.0732	3400.5905	570.1730	1872.4515	2180.6566
	18.00 %	1073.6323	446.9863	540.3370	1339.5496	3610.2968	711.4901	1860.8943	2365.8963
APC3	-18.00 %	630.9351	291.9349	201.8059	190.3276	2017.5098	552.5724	288.7456	-139.4773
	-12.00 %	694.6621	321.0803	247.8897	815.5303	2350.2262	517.3419	899.7348	767.2686
	-6.00 %	761.7198	290.3548	179.7582	1522.4231	2517.7615	529.3067	887.4074	914.8134
	0.00 %	856.3587	351.4448	349.4732	1736.2022	2879.2914	566.3985	984.5277	1062.1019
	6.00 %	938.7240	416.2865	311.5347	1554.2985	3171.3180	642.6947	1184.1891	1181.3335
	12.00 %	1083.3703	509.2525	440.9978	1876.6349	3502.9905	678.7434	2164.4493	2394.4713
	18.00 %	1185.5691	600.4207	550.3236	1470.6845	3854.2175	810.1574	1765.4585	2056.1356

Table A.62: The γ_{xxzz} values for a CO_2 molecule at a maximum field of 0.01 au.

Basis Set	Bond Length (%)	RHF Energy	RHF Dipole X	RHF Dipole Z	MP2 Energy	MP2 Dipole X	MP2 Dipole Z	CCSD Energy	CCSD(T) Energy
	-18.00 %	183.6223	182.1289	174.4156	260.0894	334.7198	385.2845	246.6203	269.8827
	-12.00 %	202.0304	204.7799	192.1979	311.6115	363.5693	404.8383	266.0526	286.3168
	-6.00 %	229.5906	234.8410	209.0484	400.8350	416.0790	430.6196	306.4777	326.8362
ACCT	0.00 %	270.2554	260.9360	260.4281	391.5555	464.9203	443.6620	348.1061	374.8139
	6.00 %	312.5443	307.5434	303.7870	413.4258	531.7614	459.0441	430.9764	443.3882
	12.00 %	368.7498	362.9574	360.6148	533.2196	594.9338	451.7116	553.7997	542.1411
	18.00 %	440.5065	429.0769	443.7632	955.6569	647.6454	491.7881	559.1939	625.4361
	-18.00 %	220.2988	215.1942	207.6614	298.8760	236.7614	458.9106	288.8740	306.2357
	-12.00 %	244.8226	238.9890	230.0529	360.6838	289.1271	485.7554	317.3212	339.5845
	-6.00 %	271.3742	268.6152	262.5319	442.8400	362.9130	509.6143	361.2738	381.1148
ACCQ	0.00 %	316.9310	311.6402	304.8599	428.9792	464.3722	533.2435	414.9800	447.8922
	6.00 %	361.8895	356.9737	359.6298	515.8300	588.4387	555.0255	511.4299	520.8183
	12.00 %	434.8867	418.7343	419.1360	629.1233	732.4819	564.4488	605.0806	650.5394
	18.00 %	510.2435	486.8480	503.8961	1083.2225	851.2561	607.5950	658.6758	730.3330
	-18.00 %	253.1289	254.0927	250.7435	344.9977	290.3898	511.2565	323.2237	358.4786
	-12.00 %	283.2027	281.2301	277.9397	422.1733	359.0387	539.5330	383.1158	406.0262
	-6.00 %	318.2531	315.1833	306.5974	505.5998	445.7120	574.3040	430.1315	459.7919
APC3	0.00 %	366.5736	363.5511	356.6811	563.7128	567.8036	607.6197	500.5058	532.3865
	6.00 %	423.3390	423.9126	420.4449	615.6552	719.3379	649.2953	592.2506	626.1291
	12.00 %	484.7094	484.0057	485.0707	717.9285	884.8157	677.0004	730.6881	785.9126
	18.00 %	586.4266	570.5433	580.5278	937.8666	1053.1455	716.0482	799.7312	856.8849

Table A.63: The γ_{xxzz} values for a CO_2 molecule at a maximum field of 0.015 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	180.6601	263.8304	240.6693	261.2771
	-12.00 %	202.6004	297.0878	268.9831	286.5272
	-6.00 %	228.1411	336.8760	309.0053	325.9840
	0.00 %	262.3348	377.6365	353.9020	380.0503
	6.00 %	307.5578	434.2613	420.6324	443.4253
	12.00 %	361.5232	505.3601	489.3955	514.3632
	18.00 %	426.7007	620.5359	569.1485	601.1322
ACCQ	-18.00 %	217.5420	310.5585	287.8177	307.1284
	-12.00 %	243.6230	356.2232	320.6508	341.4738
	-6.00 %	274.0970	405.3057	365.1403	390.2450
	0.00 %	311.0602	440.7065	420.1166	447.5666
	6.00 %	361.0356	522.4001	491.7399	522.1695
	12.00 %	421.1560	609.0030	570.7070	618.7941
	18.00 %	493.8223	743.8915	665.1354	719.5244
APC3	-18.00 %	252.7922	365.2438	333.1891	355.9983
	-12.00 %	280.2964	411.9447	374.0712	403.2278
	-6.00 %	317.4341	477.7119	429.2821	457.3643
	0.00 %	362.1326	552.5715	500.6707	537.1431
	6.00 %	419.1193	633.0081	582.3287	625.1828
	12.00 %	490.1156	736.0409	686.4566	743.5925
	18.00 %	573.8794	909.8677	804.4010	877.7065

Table A.64: The γ_{xxzz} values for a CO_2 molecule at a maximum field of 0.02 au.

Basis Set	Bond Length (%)	RHF Energy	MP2 Energy	CCSD Energy	CCSD(T) Energy
ACCT	-18.00 %	183.2625	265.0972	246.7072	261.9916
	-12.00 %	202.3899	295.4233	273.9597	292.1636
	-6.00 %	230.8481	335.6627	311.8000	332.6758
	0.00 %	265.3627	381.1854	360.4794	382.5625
	6.00 %	307.4352	439.9189	422.4235	447.0634
	12.00 %	363.3346	504.4131	492.4560	524.1158
	18.00 %	433.4635	578.8102	575.2729	611.8778
ACCQ	-18.00 %	219.5447	318.1141	290.0554	308.2914
	-12.00 %	243.5255	357.5550	323.9956	346.1953
	-6.00 %	275.3265	407.8778	368.8044	394.7939
	0.00 %	313.2615	457.4019	423.0591	455.2175
	6.00 %	361.9684	530.1581	496.6282	530.9575
	12.00 %	421.7011	612.3781	577.4961	623.3780
	18.00 %	498.6122	705.9950	675.3994	727.4776
APC3	-18.00 %	254.2840	371.1148	338.2904	362.6042
	-12.00 %	282.7576	418.0141	380.2140	407.5435
	-6.00 %	320.6490	482.6707	436.5823	468.2330
	0.00 %	369.7803	558.5535	504.8024	543.4516
	6.00 %	427.0048	646.0312	594.3492	639.1286
	12.00 %	496.5447	747.5645	696.6374	754.2241
	18.00 %	582.2495	867.7170	817.8366	889.9746

B RHF Fitting Results for All Basis Sets and ±20% of Equilibrium Bond Length

B.1 α_{xx} Results

Table B.1: Fitting coefficients and errors for the CCD basis set for the RHF α_{xx} values at zero field.

CCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.0611	0.0608	0.0609	0.0611	0.0607	0.0608
b_2	0.0611	0.0608	0.0609	0.0611	0.0607	0.0608
b_3	0.0627	0.0627	0.0627	0.0627	0.0627	0.0627
b_4	0.0627	0.0627	0.0627	0.0627	0.0627	0.0627
b_5	0.0627	0.0627	0.0627	0.0627	0.0627	0.0627
c_2	-4.55×10^{-4}	-4.50×10^{-4}	-4.51×10^{-4}	-4.56×10^{-4}	-4.49×10^{-4}	-4.50×10^{-4}
c_3	-4.55×10^{-4}	-4.50×10^{-4}	-4.51×10^{-4}	-4.56×10^{-4}	-4.49×10^{-4}	-4.50×10^{-4}
c_4	-4.89×10^{-4}	-4.88×10^{-4}	-4.88×10^{-4}	-4.89×10^{-4}	-4.88×10^{-4}	-4.88×10^{-4}
c_5	-4.89×10^{-4}	-4.88×10^{-4}	-4.88×10^{-4}	-4.89×10^{-4}	-4.88×10^{-4}	-4.88×10^{-4}
d_3	-6.22×10^{-6}	-6.25×10^{-6}	-6.24×10^{-6}	-6.20×10^{-6}	-6.25×10^{-6}	-6.25×10^{-6}
d_4	-6.22×10^{-6}	-6.25×10^{-6}	-6.24×10^{-6}	-6.20×10^{-6}	-6.25×10^{-6}	-6.25×10^{-6}
d_5	-5.97×10^{-6}	-5.96×10^{-6}	-5.97×10^{-6}	-5.92×10^{-6}	-5.95×10^{-6}	-5.96×10^{-6}
e_4	1.11×10^{-7}	1.10×10^{-7}	1.10×10^{-7}	1.15×10^{-7}	1.09×10^{-7}	1.09×10^{-7}
e_5	1.11×10^{-7}	1.10×10^{-7}	1.10×10^{-7}	1.15×10^{-7}	1.09×10^{-7}	1.09×10^{-7}
g_5	-5.53×10^{-10}	-5.53×10^{-10}	-5.41×10^{-10}	-6.75×10^{-10}	-5.73×10^{-10}	-5.48×10^{-10}
$RMSE_1$	0.0859	0.0859	0.0859	0.0859	0.0860	0.0860
$RMSE_2$	8.28×10^{-3}	8.93×10^{-3}	8.67×10^{-3}	8.28×10^{-3}	9.46×10^{-3}	9.20×10^{-3}
$RMSE_3$	1.86×10^{-3}	2.07×10^{-3}	1.99×10^{-3}	1.86×10^{-3}	2.18×10^{-3}	2.11×10^{-3}
$RMSE_4$	1.06×10^{-4}	1.21×10^{-4}	1.17×10^{-4}	1.30×10^{-4}	1.25×10^{-4}	1.22×10^{-4}
$RMSE_5$	7.49×10^{-5}	8.74×10^{-5}	8.41×10^{-5}	1.04×10^{-4}	9.00×10^{-5}	8.73×10^{-5}
Percent Error 1	2.392	2.326	2.342	2.392	2.301	2.392
Percent Error 2	0.395	0.268	0.297	0.400	0.253	0.400
Percent Error 3	0.077	0.053	0.050	0.083	0.056	0.083
Percent Error 4	3.86×10^{-3}	3.48×10^{-3}	3.22×10^{-3}	7.38×10^{-3}	3.61×10^{-3}	7.38×10^{-3}
Percent Error 5	3.15×10^{-3}	3.12×10^{-3}	2.79×10^{-3}	8.31×10^{-3}	3.35×10^{-3}	8.31×10^{-3}

Table B.2: Fitting coefficients and errors for the CCT basis set for the RHF α_{xx} values at zero field.

CCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.0875	0.0870	0.0871	0.0875	0.0868	0.0869
b_2	0.0875	0.0870	0.0871	0.0875	0.0868	0.0869
b_3	0.0902	0.0902	0.0902	0.0902	0.0902	0.0902
b_4	0.0902	0.0902	0.0902	0.0902	0.0902	0.0902
b_5	0.0902	0.0902	0.0902	0.0902	0.0902	0.0902
c_2	-4.09×10^{-4}	-4.08×10^{-4}	-4.09×10^{-4}	-4.09×10^{-4}	-4.08×10^{-4}	-4.08×10^{-4}
c_3	-4.09×10^{-4}	-4.08×10^{-4}	-4.09×10^{-4}	-4.09×10^{-4}	-4.08×10^{-4}	-4.08×10^{-4}
c_4	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}
c_5	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}	-4.12×10^{-4}
d_3	-1.09×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.08×10^{-5}	-1.08×10^{-5}
d_4	-1.09×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.08×10^{-5}	-1.08×10^{-5}
d_5	-1.11×10^{-5}	-1.11×10^{-5}	-1.11×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}	-1.11×10^{-5}
e_4	9.97×10^{-9}	9.64×10^{-9}	9.64×10^{-9}	1.08×10^{-8}	9.65×10^{-9}	9.58×10^{-9}
e_5	9.97×10^{-9}	9.64×10^{-9}	9.63×10^{-9}	1.08×10^{-8}	9.65×10^{-9}	9.58×10^{-9}
g_5	4.34×10^{-10}	4.38×10^{-10}	4.63×10^{-10}	1.33×10^{-10}	3.88×10^{-10}	4.49×10^{-10}
$RMSE_1$	0.0780	0.0782	0.0782	0.0780	0.0784	0.0783
$RMSE_2$	0.0141	0.0152	0.0147	0.0141	0.0160	0.0156
$RMSE_3$	1.79×10^{-4}	2.00×10^{-4}	1.93×10^{-4}	1.84×10^{-4}	2.10×10^{-4}	2.03×10^{-4}
$RMSE_4$	6.53×10^{-5}	8.30×10^{-5}	7.79×10^{-5}	8.10×10^{-5}	8.72×10^{-5}	8.32×10^{-5}
$RMSE_5$	2.78×10^{-5}	3.29×10^{-5}	3.11×10^{-5}	6.37×10^{-5}	3.70×10^{-5}	3.25×10^{-5}
Percent Error 1	1.791	1.705	1.726	1.790	1.673	1.790
Percent Error 2	0.434	0.307	0.337	0.434	0.276	0.434
Percent Error 3	5.03×10^{-3}	3.40×10^{-3}	3.14×10^{-3}	6.34×10^{-3}	3.65×10^{-3}	6.34×10^{-3}
Percent Error 4	2.86×10^{-3}	2.61×10^{-3}	2.41×10^{-3}	5.21×10^{-3}	2.74×10^{-3}	5.21×10^{-3}
Percent Error 5	1.04×10^{-3}	1.31×10^{-3}	1.14×10^{-3}	4.35×10^{-3}	1.53×10^{-3}	4.35×10^{-3}

Table B.3: Fitting coefficients and errors for the CCQ basis set for the RHF α_{xx} values at zero field.

CCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1083	0.1079	0.1080	0.1083	0.1077	0.1078
b_2	0.1083	0.1079	0.1080	0.1083	0.1077	0.1078
b_3	0.1109	0.1109	0.1109	0.1109	0.1109	0.1109
b_4	0.1109	0.1109	0.1109	0.1109	0.1109	0.1109
b_5	0.1109	0.1109	0.1109	0.1109	0.1109	0.1109
c_2	-2.73×10^{-4}	-2.74×10^{-4}	-2.74×10^{-4}	-2.73×10^{-4}	-2.74×10^{-4}	-2.74×10^{-4}
c_3	-2.73×10^{-4}	-2.74×10^{-4}	-2.74×10^{-4}	-2.73×10^{-4}	-2.74×10^{-4}	-2.74×10^{-4}
c_4	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}
c_5	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}	-2.67×10^{-4}
d_3	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}
d_4	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}
d_5	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}
e_4	-1.90×10^{-8}	-1.90×10^{-8}	-1.90×10^{-8}	-1.89×10^{-8}	-1.90×10^{-8}	-1.90×10^{-8}
e_5	-1.90×10^{-8}	-1.90×10^{-8}	-1.90×10^{-8}	-1.89×10^{-8}	-1.90×10^{-8}	-1.90×10^{-8}
g_5	-9.73×10^{-11}	-1.00×10^{-10}	-1.05×10^{-10}	-1.71×10^{-11}	-8.78×10^{-11}	-1.04×10^{-10}
$RMSE_1$	0.0530	0.0533	0.0532	0.0530	0.0535	0.0534
$RMSE_2$	0.0134	0.0144	0.0140	0.0134	0.0153	0.0149
$RMSE_3$	3.17×10^{-4}	3.57×10^{-4}	3.42×10^{-4}	3.19×10^{-4}	3.78×10^{-4}	3.64×10^{-4}
$RMSE_4$	1.52×10^{-5}	1.90×10^{-5}	1.79×10^{-5}	1.83×10^{-5}	2.00×10^{-5}	1.91×10^{-5}
$RMSE_5$	7.39×10^{-6}	8.15×10^{-6}	7.87×10^{-6}	1.61×10^{-5}	8.98×10^{-6}	8.05×10^{-6}
Percent Error 1	1.117	1.046	1.063	1.117	1.019	1.117
Percent Error 2	0.250	0.176	0.193	0.250	0.192	0.250
Percent Error 3	6.41×10^{-3}	4.78×10^{-3}	4.52×10^{-3}	7.10×10^{-3}	5.13×10^{-3}	7.10×10^{-3}
Percent Error 4	3.45×10^{-4}	3.25×10^{-4}	3.04×10^{-4}	5.84×10^{-4}	3.35×10^{-4}	5.84×10^{-4}
Percent Error 5	1.03×10^{-4}	1.72×10^{-4}	1.29×10^{-4}	5.18×10^{-4}	2.12×10^{-4}	5.18×10^{-4}

Table B.4: Fitting coefficients and errors for the ACCD basis set for the RHF α_{xx} values at zero field.

ACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1282	0.1277	0.1279	0.1282	0.1276	0.1276
b_2	0.1282	0.1277	0.1279	0.1282	0.1276	0.1276
b_3	0.1311	0.1311	0.1311	0.1311	0.1311	0.1311
b_4	0.1311	0.1311	0.1311	0.1311	0.1311	0.1311
b_5	0.1312	0.1312	0.1312	0.1312	0.1312	0.1312
c_2	-9.97×10^{-5}	-1.02×10^{-4}	-1.01×10^{-4}	-9.94×10^{-5}	-1.02×10^{-4}	-1.02×10^{-4}
c_3	-9.97×10^{-5}	-1.02×10^{-4}	-1.01×10^{-4}	-9.94×10^{-5}	-1.02×10^{-4}	-1.02×10^{-4}
c_4	-8.71×10^{-5}	-8.72×10^{-5}	-8.72×10^{-5}	-8.71×10^{-5}	-8.71×10^{-5}	-8.72×10^{-5}
c_5	-8.71×10^{-5}	-8.72×10^{-5}	-8.72×10^{-5}	-8.71×10^{-5}	-8.71×10^{-5}	-8.72×10^{-5}
d_3	-1.15×10^{-5}	-1.15×10^{-5}	-1.15×10^{-5}	-1.16×10^{-5}	-1.15×10^{-5}	-1.15×10^{-5}
d_4	-1.15×10^{-5}	-1.15×10^{-5}	-1.15×10^{-5}	-1.16×10^{-5}	-1.15×10^{-5}	-1.15×10^{-5}
d_5	-1.19×10^{-5}	-1.19×10^{-5}	-1.19×10^{-5}	-1.19×10^{-5}	-1.19×10^{-5}	-1.19×10^{-5}
e_4	-4.19×10^{-8}	-4.18×10^{-8}	-4.18×10^{-8}	-4.21×10^{-8}	-4.18×10^{-8}	-4.18×10^{-8}
e_5	-4.19×10^{-8}	-4.18×10^{-8}	-4.18×10^{-8}	-4.21×10^{-8}	-4.18×10^{-8}	-4.18×10^{-8}
g_5	6.67×10^{-10}	6.67×10^{-10}	6.57×10^{-10}	7.75×10^{-10}	6.83×10^{-10}	6.63×10^{-10}
$RMSE_1$	0.0240	0.0247	0.0244	0.0240	0.0253	0.0250
$RMSE_2$	0.0150	0.0161	0.0157	0.0150	0.0170	0.0166
$RMSE_3$	7.05×10^{-4}	7.92×10^{-4}	7.59×10^{-4}	7.08×10^{-4}	8.36×10^{-4}	8.07×10^{-4}
$RMSE_4$	9.15×10^{-5}	1.04×10^{-4}	9.99×10^{-5}	9.82×10^{-5}	1.07×10^{-4}	1.04×10^{-4}
$RMSE_5$	9.67×10^{-6}	1.17×10^{-5}	1.10×10^{-5}	2.27×10^{-5}	1.31×10^{-5}	1.15×10^{-5}
Percent Error 1	0.550	0.478	0.495	0.549	0.450	0.549
Percent Error 2	0.260	0.182	0.200	0.260	0.203	0.260
Percent Error 3	0.021	0.014	0.013	0.024	0.015	0.024
Percent Error 4	1.48×10^{-3}	1.27×10^{-3}	1.20×10^{-3}	2.30×10^{-3}	1.30×10^{-3}	2.30×10^{-3}
Percent Error 5	3.15×10^{-4}	4.13×10^{-4}	3.56×10^{-4}	1.32×10^{-3}	4.79×10^{-4}	1.32×10^{-3}

Table B.5: Fitting coefficients and errors for the ACCT basis set for the RHF α_{xx} values at zero field.

ACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1361	0.1356	0.1357	0.1361	0.1354	0.1355
b_2	0.1361	0.1356	0.1357	0.1361	0.1354	0.1355
b_3	0.1388	0.1388	0.1388	0.1388	0.1388	0.1388
b_4	0.1388	0.1388	0.1388	0.1388	0.1388	0.1388
b_5	0.1387	0.1387	0.1387	0.1387	0.1387	0.1387
c_2	-9.41×10^{-5}	-9.53×10^{-5}	-9.51×10^{-5}	-9.39×10^{-5}	-9.56×10^{-5}	-9.54×10^{-5}
c_3	-9.41×10^{-5}	-9.53×10^{-5}	-9.50×10^{-5}	-9.39×10^{-5}	-9.56×10^{-5}	-9.54×10^{-5}
c_4	-8.58×10^{-5}	-8.59×10^{-5}	-8.59×10^{-5}	-8.56×10^{-5}	-8.59×10^{-5}	-8.59×10^{-5}
c_5	-8.58×10^{-5}	-8.59×10^{-5}	-8.59×10^{-5}	-8.56×10^{-5}	-8.59×10^{-5}	-8.59×10^{-5}
d_3	-1.06×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}	-1.06×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}
d_4	-1.06×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}	-1.06×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}
d_5	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}	-1.03×10^{-5}
e_4	-2.77×10^{-8}	-2.73×10^{-8}	-2.74×10^{-8}	-2.84×10^{-8}	-2.73×10^{-8}	-2.73×10^{-8}
e_5	-2.77×10^{-8}	-2.73×10^{-8}	-2.74×10^{-8}	-2.84×10^{-8}	-2.73×10^{-8}	-2.73×10^{-8}
g_5	-7.76×10^{-10}	-7.75×10^{-10}	-7.73×10^{-10}	-8.06×10^{-10}	-7.83×10^{-10}	-7.74×10^{-10}
$RMSE_1$	0.0224	0.0231	0.0228	0.0224	0.0237	0.0234
$RMSE_2$	0.0138	0.0148	0.0144	0.0138	0.0157	0.0153
$RMSE_3$	4.74×10^{-4}	5.30×10^{-4}	5.09×10^{-4}	4.78×10^{-4}	5.58×10^{-4}	5.39×10^{-4}
$RMSE_4$	1.07×10^{-4}	1.23×10^{-4}	1.19×10^{-4}	1.17×10^{-4}	1.28×10^{-4}	1.24×10^{-4}
$RMSE_5$	1.58×10^{-5}	1.83×10^{-5}	1.76×10^{-5}	2.21×10^{-5}	1.89×10^{-5}	1.83×10^{-5}
Percent Error 1	0.487	0.423	0.438	0.487	0.399	0.487
Percent Error 2	0.227	0.159	0.175	0.227	0.176	0.227
Percent Error 3	9.11×10^{-3}	6.79×10^{-3}	6.36×10^{-3}	0.011	7.20×10^{-3}	0.011
Percent Error 4	2.99×10^{-3}	2.40×10^{-3}	2.22×10^{-3}	4.89×10^{-3}	2.50×10^{-3}	4.89×10^{-3}
Percent Error 5	2.65×10^{-4}	2.73×10^{-4}	2.52×10^{-4}	7.24×10^{-4}	3.02×10^{-4}	7.24×10^{-4}

Table B.6: Fitting coefficients and errors for the ACCQ basis set for the RHF α_{xx} values at zero field.

ACCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1390	0.1385	0.1386	0.1390	0.1383	0.1384
b_2	0.1390	0.1385	0.1386	0.1390	0.1383	0.1384
b_3	0.1417	0.1417	0.1417	0.1417	0.1417	0.1417
b_4	0.1417	0.1417	0.1417	0.1417	0.1417	0.1417
b_5	0.1417	0.1417	0.1417	0.1417	0.1417	0.1417
c_2	-8.47×10^{-5}	-8.53×10^{-5}	-8.52×10^{-5}	-8.46×10^{-5}	-8.55×10^{-5}	-8.54×10^{-5}
c_3	-8.47×10^{-5}	-8.53×10^{-5}	-8.52×10^{-5}	-8.46×10^{-5}	-8.55×10^{-5}	-8.54×10^{-5}
c_4	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}
c_5	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}	-8.04×10^{-5}
d_3	-1.09×10^{-5}	-1.10×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}
d_4	-1.09×10^{-5}	-1.10×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}
d_5	-1.06×10^{-5}	-1.06×10^{-5}	-1.06×10^{-5}	-1.07×10^{-5}	-1.06×10^{-5}	-1.06×10^{-5}
e_4	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}
e_5	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}	-1.42×10^{-8}
g_5	-5.88×10^{-10}	-5.88×10^{-10}	-5.90×10^{-10}	-5.82×10^{-10}	-5.89×10^{-10}	-5.88×10^{-10}
$RMSE_1$	0.0213	0.0220	0.0217	0.0213	0.0227	0.0224
$RMSE_2$	0.0142	0.0152	0.0148	0.0142	0.0162	0.0157
$RMSE_3$	2.50×10^{-4}	2.82×10^{-4}	2.70×10^{-4}	2.53×10^{-4}	2.98×10^{-4}	2.87×10^{-4}
$RMSE_4$	8.03×10^{-5}	9.34×10^{-5}	8.94×10^{-5}	8.84×10^{-5}	9.70×10^{-5}	9.39×10^{-5}
$RMSE_5$	2.98×10^{-6}	3.01×10^{-6}	3.01×10^{-6}	3.18×10^{-6}	3.09×10^{-6}	3.00×10^{-6}
Percent Error 1	0.457	0.392	0.408	0.457	0.368	0.457
Percent Error 2	0.226	0.159	0.175	0.226	0.176	0.226
Percent Error 3	5.15×10^{-3}	3.77×10^{-3}	3.53×10^{-3}	6.15×10^{-3}	3.98×10^{-3}	6.15×10^{-3}
Percent Error 4	1.26×10^{-3}	1.11×10^{-3}	1.04×10^{-3}	3.15×10^{-3}	1.67×10^{-3}	3.15×10^{-3}
Percent Error 5	4.80×10^{-5}	4.94×10^{-5}	5.04×10^{-5}	4.72×10^{-5}	5.17×10^{-5}	4.72×10^{-5}

Table B.7: Fitting coefficients and errors for the DACCD basis set for the RHF α_{xx} values at zero field.

DACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1396	0.1391	0.1392	0.1396	0.1389	0.1390
b_2	0.1396	0.1391	0.1392	0.1396	0.1389	0.1390
b_3	0.1425	0.1425	0.1425	0.1425	0.1425	0.1425
b_4	0.1425	0.1425	0.1425	0.1425	0.1425	0.1425
b_5	0.1425	0.1425	0.1425	0.1425	0.1425	0.1425
c_2	-9.77×10^{-5}	-9.74×10^{-5}	-9.75×10^{-5}	-9.77×10^{-5}	-9.73×10^{-5}	-9.73×10^{-5}
c_3	-9.77×10^{-5}	-9.74×10^{-5}	-9.75×10^{-5}	-9.77×10^{-5}	-9.73×10^{-5}	-9.74×10^{-5}
c_4	-1.00×10^{-4}	-1.00×10^{-4}	-1.00×10^{-4}	-1.01×10^{-4}	-1.00×10^{-4}	-1.00×10^{-4}
c_5	-1.00×10^{-4}	-1.00×10^{-4}	-1.00×10^{-4}	-1.01×10^{-4}	-1.00×10^{-4}	-1.00×10^{-4}
d_3	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}
d_4	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}
d_5	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}	-1.14×10^{-5}
e_4	9.34×10^{-9}	8.47×10^{-9}	8.52×10^{-9}	1.13×10^{-8}	8.38×10^{-9}	8.30×10^{-9}
e_5	9.34×10^{-9}	8.47×10^{-9}	8.52×10^{-9}	1.13×10^{-8}	8.38×10^{-9}	8.30×10^{-9}
g_5	6.45×10^{-12}	5.23×10^{-12}	9.55×10^{-12}	-1.45×10^{-11}	2.62×10^{-12}	2.70×10^{-12}
$RMSE_1$	0.0235	0.0242	0.0240	0.0235	0.0249	0.0246
$RMSE_2$	0.0147	0.0159	0.0154	0.0147	0.0168	0.0163
$RMSE_3$	1.61×10^{-4}	1.70×10^{-4}	1.67×10^{-4}	1.61×10^{-4}	1.76×10^{-4}	1.73×10^{-4}
$RMSE_4$	3.97×10^{-5}	4.59×10^{-5}	4.43×10^{-5}	5.36×10^{-5}	4.71×10^{-5}	4.59×10^{-5}
$RMSE_5$	3.97×10^{-5}	4.59×10^{-5}	4.43×10^{-5}	5.37×10^{-5}	4.71×10^{-5}	4.59×10^{-5}
Percent Error 1	0.494	0.427	0.443	0.494	0.402	0.494
Percent Error 2	0.371	0.263	0.288	0.371	0.231	0.371
Percent Error 3	2.02×10^{-3}	2.64×10^{-3}	2.57×10^{-3}	2.06×10^{-3}	2.78×10^{-3}	2.06×10^{-3}
Percent Error 4	9.89×10^{-4}	9.40×10^{-4}	8.77×10^{-4}	2.28×10^{-3}	9.68×10^{-4}	2.28×10^{-3}
Percent Error 5	9.67×10^{-4}	9.26×10^{-4}	8.53×10^{-4}	2.35×10^{-3}	9.61×10^{-4}	2.35×10^{-3}

Table B.8: Fitting coefficients and errors for the DACCT basis set for the RHF α_{xx} values at zero field.

DACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1398	0.1394	0.1395	0.1398	0.1392	0.1393
b_2	0.1398	0.1394	0.1395	0.1398	0.1392	0.1393
b_3	0.1426	0.1426	0.1426	0.1426	0.1426	0.1426
b_4	0.1426	0.1426	0.1426	0.1426	0.1426	0.1426
b_5	0.1426	0.1426	0.1426	0.1426	0.1426	0.1426
c_2	-7.29×10^{-5}	-7.38×10^{-5}	-7.36×10^{-5}	-7.28×10^{-5}	-7.40×10^{-5}	-7.39×10^{-5}
c_3	-7.29×10^{-5}	-7.38×10^{-5}	-7.36×10^{-5}	-7.28×10^{-5}	-7.40×10^{-5}	-7.39×10^{-5}
c_4	-6.69×10^{-5}	-6.70×10^{-5}	-6.70×10^{-5}	-6.68×10^{-5}	-6.70×10^{-5}	-6.70×10^{-5}
c_5	-6.69×10^{-5}	-6.70×10^{-5}	-6.70×10^{-5}	-6.68×10^{-5}	-6.70×10^{-5}	-6.70×10^{-5}
d_3	-1.10×10^{-5}	-1.11×10^{-5}	-1.11×10^{-5}	-1.10×10^{-5}	-1.11×10^{-5}	-1.11×10^{-5}
d_4	-1.10×10^{-5}	-1.11×10^{-5}	-1.11×10^{-5}	-1.10×10^{-5}	-1.11×10^{-5}	-1.11×10^{-5}
d_5	-1.08×10^{-5}	-1.08×10^{-5}	-1.08×10^{-5}	-1.08×10^{-5}	-1.08×10^{-5}	-1.08×10^{-5}
e_4	-2.01×10^{-8}	-1.98×10^{-8}	-1.99×10^{-8}	-2.05×10^{-8}	-1.98×10^{-8}	-1.98×10^{-8}
e_5	-2.01×10^{-8}	-1.98×10^{-8}	-1.99×10^{-8}	-2.05×10^{-8}	-1.98×10^{-8}	-1.98×10^{-8}
g_5	-5.47×10^{-10}	-5.48×10^{-10}	-5.49×10^{-10}	-5.45×10^{-10}	-5.50×10^{-10}	-5.50×10^{-10}
$RMSE_1$	0.0198	0.0206	0.0203	0.0198	0.0213	0.0210
$RMSE_2$	0.0143	0.0154	0.0150	0.0143	0.0163	0.0159
$RMSE_3$	3.43×10^{-4}	3.84×10^{-4}	3.69×10^{-4}	3.46×10^{-4}	4.05×10^{-4}	3.91×10^{-4}
$RMSE_4$	7.53×10^{-5}	8.75×10^{-5}	8.38×10^{-5}	8.31×10^{-5}	9.09×10^{-5}	8.79×10^{-5}
$RMSE_5$	9.75×10^{-6}	1.13×10^{-5}	1.09×10^{-5}	1.33×10^{-5}	1.16×10^{-5}	1.13×10^{-5}
Percent Error 1	0.427	0.362	0.378	0.427	0.337	0.427
Percent Error 2	0.229	0.161	0.177	0.229	0.178	0.229
Percent Error 3	6.51×10^{-3}	4.83×10^{-3}	4.52×10^{-3}	7.52×10^{-3}	5.13×10^{-3}	7.52×10^{-3}
Percent Error 4	2.10×10^{-3}	1.70×10^{-3}	1.56×10^{-3}	3.43×10^{-3}	1.77×10^{-3}	3.43×10^{-3}
Percent Error 5	1.44×10^{-4}	1.43×10^{-4}	1.36×10^{-4}	3.39×10^{-4}	1.55×10^{-4}	3.39×10^{-4}

Table B.9: Fitting coefficients and errors for the PC3 basis set for the RHF α_{xx} values at zero field.

PC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1239	0.1235	0.1236	0.1239	0.1233	0.1234
b_2	0.1239	0.1235	0.1236	0.1239	0.1233	0.1234
b_3	0.1263	0.1263	0.1263	0.1263	0.1264	0.1264
b_4	0.1263	0.1263	0.1263	0.1263	0.1264	0.1264
b_5	0.1263	0.1263	0.1263	0.1263	0.1263	0.1263
c_2	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}
c_3	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}	-1.88×10^{-4}
c_4	-1.87×10^{-4}	-1.87×10^{-4}	-1.87×10^{-4}	-1.88×10^{-4}	-1.87×10^{-4}	-1.87×10^{-4}
c_5	-1.87×10^{-4}	-1.87×10^{-4}	-1.87×10^{-4}	-1.88×10^{-4}	-1.87×10^{-4}	-1.87×10^{-4}
d_3	-9.72×10^{-6}	-9.76×10^{-6}	-9.75×10^{-6}	-9.68×10^{-6}	-9.77×10^{-6}	-9.76×10^{-6}
d_4	-9.72×10^{-6}	-9.76×10^{-6}	-9.75×10^{-6}	-9.68×10^{-6}	-9.77×10^{-6}	-9.76×10^{-6}
d_5	-9.29×10^{-6}	-9.29×10^{-6}	-9.29×10^{-6}	-9.26×10^{-6}	-9.28×10^{-6}	-9.29×10^{-6}
e_4	-1.38×10^{-9}	-1.62×10^{-9}	-1.62×10^{-9}	-8.42×10^{-10}	-1.67×10^{-9}	-1.67×10^{-9}
e_5	-1.38×10^{-9}	-1.62×10^{-9}	-1.61×10^{-9}	-8.42×10^{-10}	-1.67×10^{-9}	-1.68×10^{-9}
g_5	-9.19×10^{-10}	-9.17×10^{-10}	-9.12×10^{-10}	-9.95×10^{-10}	-9.29×10^{-10}	-9.14×10^{-10}
$RMSE_1$	0.0374	0.0378	0.0376	0.0374	0.0381	0.0379
$RMSE_2$	0.0126	0.0136	0.0132	0.0126	0.0144	0.0140
$RMSE_3$	1.28×10^{-4}	1.48×10^{-4}	1.42×10^{-4}	1.39×10^{-4}	1.53×10^{-4}	1.48×10^{-4}
$RMSE_4$	1.26×10^{-4}	1.45×10^{-4}	1.39×10^{-4}	1.37×10^{-4}	1.50×10^{-4}	1.45×10^{-4}
$RMSE_5$	1.43×10^{-5}	1.61×10^{-5}	1.56×10^{-5}	2.23×10^{-5}	1.68×10^{-5}	1.61×10^{-5}
Percent Error 1	0.760	0.698	0.712	0.760	0.674	0.760
Percent Error 2	0.212	0.150	0.165	0.212	0.164	0.212
Percent Error 3	2.60×10^{-3}	2.19×10^{-3}	2.04×10^{-3}	3.75×10^{-3}	2.25×10^{-3}	3.75×10^{-3}
Percent Error 4	2.19×10^{-3}	1.91×10^{-3}	1.79×10^{-3}	3.49×10^{-3}	1.92×10^{-3}	3.49×10^{-3}
Percent Error 5	4.01×10^{-4}	4.03×10^{-4}	3.62×10^{-4}	1.31×10^{-3}	4.50×10^{-4}	1.31×10^{-3}

Table B.10: Fitting coefficients and errors for the APC3 basis set for the RHF α_{xx} values at zero field.

APC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1394	0.1390	0.1391	0.1394	0.1388	0.1389
b_2	0.1394	0.1390	0.1391	0.1394	0.1388	0.1389
b_3	0.1422	0.1422	0.1422	0.1422	0.1422	0.1422
b_4	0.1422	0.1422	0.1422	0.1422	0.1422	0.1422
b_5	0.1422	0.1422	0.1422	0.1422	0.1422	0.1422
c_2	-7.36×10^{-5}	-7.42×10^{-5}	-7.41×10^{-5}	-7.35×10^{-5}	-7.44×10^{-5}	-7.43×10^{-5}
c_3	-7.36×10^{-5}	-7.42×10^{-5}	-7.41×10^{-5}	-7.35×10^{-5}	-7.44×10^{-5}	-7.43×10^{-5}
c_4	-6.96×10^{-5}	-6.95×10^{-5}	-6.95×10^{-5}	-6.97×10^{-5}	-6.95×10^{-5}	-6.95×10^{-5}
c_5	-6.96×10^{-5}	-6.95×10^{-5}	-6.95×10^{-5}	-6.97×10^{-5}	-6.95×10^{-5}	-6.95×10^{-5}
d_3	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}
d_4	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}
d_5	-1.07×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}	-1.07×10^{-5}
e_4	-1.34×10^{-8}	-1.36×10^{-8}	-1.36×10^{-8}	-1.30×10^{-8}	-1.36×10^{-8}	-1.36×10^{-8}
e_5	-1.34×10^{-8}	-1.36×10^{-8}	-1.35×10^{-8}	-1.30×10^{-8}	-1.36×10^{-8}	-1.36×10^{-8}
g_5	-6.10×10^{-10}	-6.09×10^{-10}	-6.04×10^{-10}	-6.77×10^{-10}	-6.20×10^{-10}	-6.07×10^{-10}
$RMSE_1$	0.0199	0.0206	0.0203	0.0199	0.0213	0.0210
$RMSE_2$	0.0143	0.0153	0.0149	0.0143	0.0163	0.0158
$RMSE_3$	2.38×10^{-4}	2.71×10^{-4}	2.59×10^{-4}	2.42×10^{-4}	2.87×10^{-4}	2.76×10^{-4}
$RMSE_4$	8.37×10^{-5}	9.55×10^{-5}	9.19×10^{-5}	9.07×10^{-5}	9.90×10^{-5}	9.60×10^{-5}
$RMSE_5$	9.83×10^{-6}	1.14×10^{-5}	1.09×10^{-5}	1.75×10^{-5}	1.22×10^{-5}	1.13×10^{-5}
Percent Error 1	0.427	0.362	0.378	0.427	0.338	0.427
Percent Error 2	0.227	0.160	0.176	0.227	0.177	0.227
Percent Error 3	5.01×10^{-3}	3.67×10^{-3}	3.45×10^{-3}	5.97×10^{-3}	3.92×10^{-3}	5.97×10^{-3}
Percent Error 4	1.35×10^{-3}	1.17×10^{-3}	1.11×10^{-3}	2.13×10^{-3}	1.19×10^{-3}	2.13×10^{-3}
Percent Error 5	3.00×10^{-4}	3.27×10^{-4}	2.89×10^{-4}	1.04×10^{-3}	3.68×10^{-4}	1.04×10^{-3}

Table B.11: Fitting coefficients and errors for the APC4 basis set for the RHF α_{xx} values at zero field.

APC4	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.1397	0.1392	0.1393	0.1397	0.1390	0.1391
b_2	0.1397	0.1392	0.1393	0.1397	0.1390	0.1391
b_3	0.1424	0.1424	0.1424	0.1424	0.1424	0.1424
b_4	0.1424	0.1424	0.1424	0.1424	0.1424	0.1424
b_5	0.1424	0.1424	0.1424	0.1424	0.1424	0.1424
c_2	-7.57×10^{-5}	-7.64×10^{-5}	-7.63×10^{-5}	-7.56×10^{-5}	-7.66×10^{-5}	-7.65×10^{-5}
c_3	-7.57×10^{-5}	-7.64×10^{-5}	-7.62×10^{-5}	-7.56×10^{-5}	-7.66×10^{-5}	-7.65×10^{-5}
c_4	-7.07×10^{-5}	-7.07×10^{-5}	-7.07×10^{-5}	-7.06×10^{-5}	-7.07×10^{-5}	-7.07×10^{-5}
c_5	-7.07×10^{-5}	-7.07×10^{-5}	-7.07×10^{-5}	-7.06×10^{-5}	-7.07×10^{-5}	-7.07×10^{-5}
d_3	-1.09×10^{-5}	-1.10×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}
d_4	-1.09×10^{-5}	-1.10×10^{-5}	-1.09×10^{-5}	-1.09×10^{-5}	-1.10×10^{-5}	-1.10×10^{-5}
d_5	-1.06×10^{-5}	-1.06×10^{-5}	-1.06×10^{-5}	-1.06×10^{-5}	-1.06×10^{-5}	-1.06×10^{-5}
e_4	-1.67×10^{-8}	-1.66×10^{-8}	-1.66×10^{-8}	-1.70×10^{-8}	-1.66×10^{-8}	-1.66×10^{-8}
e_5	-1.67×10^{-8}	-1.66×10^{-8}	-1.66×10^{-8}	-1.70×10^{-8}	-1.66×10^{-8}	-1.66×10^{-8}
g_5	-6.40×10^{-10}	-6.44×10^{-10}	-6.44×10^{-10}	-6.64×10^{-10}	-6.48×10^{-10}	-6.43×10^{-10}
$RMSE_1$	0.0201	0.0208	0.0205	0.0201	0.0215	0.0212
$RMSE_2$	0.0142	0.0152	0.0148	0.0142	0.0162	0.0157
$RMSE_3$	2.92×10^{-4}	3.28×10^{-4}	3.15×10^{-4}	2.96×10^{-4}	3.46×10^{-4}	3.34×10^{-4}
$RMSE_4$	8.74×10^{-5}	1.00×10^{-4}	9.64×10^{-5}	9.52×10^{-5}	1.04×10^{-4}	1.01×10^{-4}
$RMSE_5$	5.48×10^{-6}	7.27×10^{-6}	7.15×10^{-6}	9.95×10^{-6}	7.80×10^{-6}	7.21×10^{-6}
Percent Error 1	0.432	0.367	0.383	0.432	0.343	0.432
Percent Error 2	0.226	0.159	0.175	0.226	0.176	0.226
Percent Error 3	5.82×10^{-3}	4.33×10^{-3}	4.06×10^{-3}	6.81×10^{-3}	4.53×10^{-3}	6.81×10^{-3}
Percent Error 4	2.24×10^{-3}	1.79×10^{-3}	1.66×10^{-3}	3.56×10^{-3}	1.86×10^{-3}	3.56×10^{-3}
Percent Error 5	1.35×10^{-4}	2.03×10^{-4}	2.01×10^{-4}	3.97×10^{-4}	2.21×10^{-4}	3.97×10^{-4}

B.2 α_{zz} Results

Table B.12: Fitting coefficients and errors for the CCD basis set for the RHF α_{zz} values at zero field.

CCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.417	0.416	0.416	0.417	0.416	0.416
b_2	0.417	0.416	0.416	0.417	0.416	0.416
b_3	0.422	0.422	0.422	0.423	0.422	0.422
b_4	0.422	0.422	0.422	0.423	0.422	0.422
b_5	0.423	0.423	0.423	0.423	0.423	0.423
c_2	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}
c_3	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}	2.31×10^{-3}
c_4	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}
c_5	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}	2.30×10^{-3}
d_3	-2.16×10^{-5}	-2.09×10^{-5}	-2.10×10^{-5}	-2.21×10^{-5}	-2.08×10^{-5}	-2.09×10^{-5}
d_4	-2.16×10^{-5}	-2.09×10^{-5}	-2.10×10^{-5}	-2.21×10^{-5}	-2.08×10^{-5}	-2.09×10^{-5}
d_5	-2.72×10^{-5}	-2.72×10^{-5}	-2.72×10^{-5}	-2.70×10^{-5}	-2.72×10^{-5}	-2.72×10^{-5}
e_4	3.06×10^{-8}	4.08×10^{-8}	4.06×10^{-8}	7.90×10^{-9}	4.16×10^{-8}	4.29×10^{-8}
e_5	3.06×10^{-8}	4.08×10^{-8}	4.06×10^{-8}	7.90×10^{-9}	4.16×10^{-8}	4.29×10^{-8}
g_5	1.22×10^{-8}	1.22×10^{-8}	1.22×10^{-8}	1.17×10^{-8}	1.21×10^{-8}	1.22×10^{-8}
$RMSE_1$	0.434	0.434	0.434	0.434	0.434	0.434
$RMSE_2$	0.028	0.030	0.029	0.028	0.031	0.031
$RMSE_3$	1.80×10^{-3}	2.14×10^{-3}	2.03×10^{-3}	1.98×10^{-3}	2.25×10^{-3}	2.15×10^{-3}
$RMSE_4$	1.72×10^{-3}	2.02×10^{-3}	1.93×10^{-3}	1.95×10^{-3}	2.10×10^{-3}	2.03×10^{-3}
$RMSE_5$	4.60×10^{-4}	5.38×10^{-4}	5.18×10^{-4}	6.38×10^{-4}	5.53×10^{-4}	5.37×10^{-4}
Percent Error 1	7.733	7.599	7.630	7.728	7.547	7.728
Percent Error 2	0.489	0.345	0.379	0.488	0.283	0.488
Percent Error 3	0.021	0.018	0.017	0.030	0.019	0.030
Percent Error 4	0.017	0.015	0.014	0.029	0.016	0.029
Percent Error 5	3.73×10^{-3}	3.94×10^{-3}	3.61×10^{-3}	9.53×10^{-3}	4.12×10^{-3}	9.53×10^{-3}

Table B.13: Fitting coefficients and errors for the CCT basis set for the RHF α_{zz} values at zero field.

CCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.425	0.424	0.424	0.425	0.424	0.424
b_2	0.425	0.424	0.424	0.425	0.424	0.424
b_3	0.432	0.432	0.432	0.432	0.432	0.432
b_4	0.432	0.432	0.432	0.432	0.432	0.432
b_5	0.433	0.433	0.433	0.433	0.433	0.433
c_2	2.57×10^{-3}	2.58×10^{-3}	2.58×10^{-3}	2.57×10^{-3}	2.58×10^{-3}	2.58×10^{-3}
c_3	2.57×10^{-3}	2.58×10^{-3}	2.58×10^{-3}	2.57×10^{-3}	2.58×10^{-3}	2.58×10^{-3}
c_4	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}
c_5	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}	2.52×10^{-3}
d_3	-2.73×10^{-5}	-2.65×10^{-5}	-2.66×10^{-5}	-2.80×10^{-5}	-2.64×10^{-5}	-2.64×10^{-5}
d_4	-2.73×10^{-5}	-2.65×10^{-5}	-2.66×10^{-5}	-2.80×10^{-5}	-2.64×10^{-5}	-2.64×10^{-5}
d_5	-3.42×10^{-5}	-3.41×10^{-5}	-3.42×10^{-5}	-3.35×10^{-5}	-3.40×10^{-5}	-3.42×10^{-5}
e_4	1.75×10^{-7}	1.77×10^{-7}	1.77×10^{-7}	1.70×10^{-7}	1.77×10^{-7}	1.77×10^{-7}
e_5	1.75×10^{-7}	1.77×10^{-7}	1.77×10^{-7}	1.70×10^{-7}	1.77×10^{-7}	1.77×10^{-7}
g_5	1.48×10^{-8}	1.48×10^{-8}	1.50×10^{-8}	1.29×10^{-8}	1.45×10^{-8}	1.49×10^{-8}
$RMSE_1$	0.484	0.484	0.484	0.484	0.484	0.484
$RMSE_2$	0.036	0.038	0.037	0.036	0.040	0.039
$RMSE_3$	3.56×10^{-3}	4.10×10^{-3}	3.91×10^{-3}	3.72×10^{-3}	4.32×10^{-3}	4.16×10^{-3}
$RMSE_4$	2.03×10^{-3}	2.41×10^{-3}	2.30×10^{-3}	2.29×10^{-3}	2.51×10^{-3}	2.42×10^{-3}
$RMSE_5$	1.76×10^{-4}	2.09×10^{-4}	1.98×10^{-4}	4.01×10^{-4}	2.35×10^{-4}	2.06×10^{-4}
Percent Error 1	7.651	7.503	7.538	7.646	7.445	7.646
Percent Error 2	0.573	0.402	0.441	0.572	0.345	0.572
Percent Error 3	0.039	0.029	0.027	0.050	0.030	0.050
Percent Error 4	0.016	0.015	0.014	0.027	0.015	0.027
Percent Error 5	1.57×10^{-3}	2.05×10^{-3}	1.79×10^{-3}	6.48×10^{-3}	2.40×10^{-3}	6.48×10^{-3}

Table B.14: Fitting coefficients and errors for the CCQ basis set for the RHF α_{zz} values at zero field.

CCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.434	0.433	0.433	0.434	0.433	0.433
b_2	0.434	0.433	0.433	0.434	0.433	0.433
b_3	0.440	0.440	0.440	0.440	0.440	0.440
b_4	0.440	0.440	0.440	0.440	0.440	0.440
b_5	0.441	0.441	0.441	0.441	0.441	0.441
c_2	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}
c_3	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}	2.67×10^{-3}
c_4	2.69×10^{-3}	2.69×10^{-3}	2.69×10^{-3}	2.70×10^{-3}	2.69×10^{-3}	2.69×10^{-3}
c_5	2.69×10^{-3}	2.69×10^{-3}	2.69×10^{-3}	2.70×10^{-3}	2.69×10^{-3}	2.69×10^{-3}
d_3	-2.45×10^{-5}	-2.37×10^{-5}	-2.38×10^{-5}	-2.53×10^{-5}	-2.36×10^{-5}	-2.36×10^{-5}
d_4	-2.45×10^{-5}	-2.37×10^{-5}	-2.38×10^{-5}	-2.53×10^{-5}	-2.36×10^{-5}	-2.36×10^{-5}
d_5	-3.23×10^{-5}	-3.23×10^{-5}	-3.23×10^{-5}	-3.22×10^{-5}	-3.23×10^{-5}	-3.23×10^{-5}
e_4	-8.00×10^{-8}	-6.41×10^{-8}	-6.46×10^{-8}	-1.15×10^{-7}	-6.28×10^{-8}	-6.09×10^{-8}
e_5	-8.00×10^{-8}	-6.41×10^{-8}	-6.46×10^{-8}	-1.15×10^{-7}	-6.28×10^{-8}	-6.09×10^{-8}
g_5	1.66×10^{-8}	1.66×10^{-8}	1.67×10^{-8}	1.64×10^{-8}	1.66×10^{-8}	1.67×10^{-8}
$RMSE_1$	0.502	0.502	0.502	0.502	0.503	0.503
$RMSE_2$	0.032	0.034	0.033	0.032	0.036	0.035
$RMSE_3$	2.73×10^{-3}	3.06×10^{-3}	2.96×10^{-3}	2.93×10^{-3}	3.15×10^{-3}	3.07×10^{-3}
$RMSE_4$	2.38×10^{-3}	2.77×10^{-3}	2.66×10^{-3}	2.69×10^{-3}	2.88×10^{-3}	2.79×10^{-3}
$RMSE_5$	7.16×10^{-4}	8.35×10^{-4}	8.05×10^{-4}	9.78×10^{-4}	8.57×10^{-4}	8.34×10^{-4}
Percent Error 1	7.396	7.271	7.300	7.391	7.223	7.391
Percent Error 2	0.212	0.186	0.166	0.209	0.196	0.209
Percent Error 3	0.045	0.019	0.019	0.062	0.020	0.062
Percent Error 4	0.021	0.019	0.018	0.036	0.020	0.036
Percent Error 5	4.93×10^{-3}	5.13×10^{-3}	4.73×10^{-3}	1.18×10^{-2}	5.33×10^{-3}	1.18×10^{-2}

Table B.15: Fitting coefficients and errors for the ACCD basis set for the RHF α_{zz} values at zero field.

ACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.440	0.439	0.440	0.440	0.439	0.439
b_2	0.440	0.439	0.440	0.440	0.439	0.439
b_3	0.446	0.446	0.446	0.446	0.446	0.446
b_4	0.446	0.446	0.446	0.446	0.446	0.446
b_5	0.446	0.446	0.446	0.446	0.446	0.446
c_2	2.52×10^{-3}	2.53×10^{-3}	2.53×10^{-3}	2.52×10^{-3}	2.53×10^{-3}	2.53×10^{-3}
c_3	2.52×10^{-3}	2.53×10^{-3}	2.53×10^{-3}	2.52×10^{-3}	2.53×10^{-3}	2.53×10^{-3}
c_4	2.49×10^{-3}	2.49×10^{-3}	2.49×10^{-3}	2.50×10^{-3}	2.49×10^{-3}	2.49×10^{-3}
c_5	2.49×10^{-3}	2.49×10^{-3}	2.49×10^{-3}	2.50×10^{-3}	2.49×10^{-3}	2.49×10^{-3}
d_3	-2.12×10^{-5}	-2.05×10^{-5}	-2.06×10^{-5}	-2.18×10^{-5}	-2.04×10^{-5}	-2.05×10^{-5}
d_4	-2.12×10^{-5}	-2.05×10^{-5}	-2.06×10^{-5}	-2.18×10^{-5}	-2.04×10^{-5}	-2.05×10^{-5}
d_5	-2.72×10^{-5}	-2.72×10^{-5}	-2.73×10^{-5}	-2.69×10^{-5}	-2.71×10^{-5}	-2.72×10^{-5}
e_4	9.93×10^{-8}	1.11×10^{-7}	1.11×10^{-7}	7.38×10^{-8}	1.12×10^{-7}	1.13×10^{-7}
e_5	9.93×10^{-8}	1.11×10^{-7}	1.11×10^{-7}	7.38×10^{-8}	1.12×10^{-7}	1.13×10^{-7}
g_5	1.30×10^{-8}	1.30×10^{-8}	1.31×10^{-8}	1.21×10^{-8}	1.29×10^{-8}	1.31×10^{-8}
$RMSE_1$	0.475	0.475	0.475	0.475	0.475	0.475
$RMSE_2$	0.028	0.029	0.029	0.028	0.031	0.030
$RMSE_3$	2.49×10^{-3}	2.97×10^{-3}	2.81×10^{-3}	2.66×10^{-3}	3.15×10^{-3}	3.01×10^{-3}
$RMSE_4$	1.85×10^{-3}	2.18×10^{-3}	2.08×10^{-3}	2.11×10^{-3}	2.27×10^{-3}	2.19×10^{-3}
$RMSE_5$	5.25×10^{-4}	6.13×10^{-4}	5.90×10^{-4}	7.37×10^{-4}	6.32×10^{-4}	6.13×10^{-4}
Percent Error 1	6.745	6.641	6.665	6.741	6.600	6.741
Percent Error 2	0.400	0.280	0.308	0.401	0.239	0.401
Percent Error 3	0.028	0.022	0.020	0.038	0.024	0.038
Percent Error 4	0.016	0.015	0.014	0.028	0.015	0.028
Percent Error 5	3.87×10^{-3}	4.07×10^{-3}	3.73×10^{-3}	1.03×10^{-2}	4.38×10^{-3}	1.03×10^{-2}

Table B.16: Fitting coefficients and errors for the ACCT basis set for the RHF α_{zz} values at zero field.

ACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.449	0.448	0.449	0.449	0.448	0.448
b_2	0.449	0.448	0.449	0.449	0.448	0.448
b_3	0.456	0.455	0.456	0.456	0.455	0.455
b_4	0.456	0.455	0.456	0.456	0.455	0.455
b_5	0.456	0.456	0.456	0.456	0.456	0.456
c_2	2.72×10^{-3}	2.73×10^{-3}	2.72×10^{-3}	2.72×10^{-3}	2.73×10^{-3}	2.73×10^{-3}
c_3	2.72×10^{-3}	2.73×10^{-3}	2.72×10^{-3}	2.72×10^{-3}	2.73×10^{-3}	2.73×10^{-3}
c_4	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.72×10^{-3}	2.71×10^{-3}	2.71×10^{-3}
c_5	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.72×10^{-3}	2.71×10^{-3}	2.71×10^{-3}
d_3	-2.48×10^{-5}	-2.40×10^{-5}	-2.41×10^{-5}	-2.54×10^{-5}	-2.39×10^{-5}	-2.40×10^{-5}
d_4	-2.48×10^{-5}	-2.40×10^{-5}	-2.41×10^{-5}	-2.54×10^{-5}	-2.39×10^{-5}	-2.40×10^{-5}
d_5	-3.14×10^{-5}	-3.14×10^{-5}	-3.14×10^{-5}	-3.11×10^{-5}	-3.13×10^{-5}	-3.14×10^{-5}
e_4	4.03×10^{-8}	5.43×10^{-8}	5.39×10^{-8}	9.51×10^{-9}	5.54×10^{-8}	5.71×10^{-8}
e_5	4.03×10^{-8}	5.43×10^{-8}	5.39×10^{-8}	9.51×10^{-9}	5.54×10^{-8}	5.71×10^{-8}
g_5	1.43×10^{-8}	1.43×10^{-8}	1.44×10^{-8}	1.36×10^{-8}	1.42×10^{-8}	1.44×10^{-8}
$RMSE_1$	0.512	0.512	0.512	0.512	0.512	0.512
$RMSE_2$	0.032	0.034	0.033	0.032	0.036	0.035
$RMSE_3$	2.16×10^{-3}	2.59×10^{-3}	2.45×10^{-3}	2.38×10^{-3}	2.72×10^{-3}	2.60×10^{-3}
$RMSE_4$	2.05×10^{-3}	2.41×10^{-3}	2.30×10^{-3}	2.34×10^{-3}	2.50×10^{-3}	2.42×10^{-3}
$RMSE_5$	6.29×10^{-4}	7.35×10^{-4}	7.08×10^{-4}	8.71×10^{-4}	7.56×10^{-4}	7.34×10^{-4}
Percent Error 1	7.330	7.207	7.236	7.326	7.159	7.326
Percent Error 2	0.453	0.320	0.351	0.453	0.271	0.453
Percent Error 3	0.023	0.020	0.018	0.032	0.020	0.032
Percent Error 4	0.018	0.016	0.015	0.031	0.017	0.031
Percent Error 5	4.45×10^{-3}	4.69×10^{-3}	4.29×10^{-3}	0.011	4.91×10^{-3}	0.011

Table B.17: Fitting coefficients and errors for the ACCQ basis set for the RHF α_{zz} values at zero field.

ACCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.449	0.448	0.449	0.449	0.448	0.448
b_2	0.449	0.448	0.449	0.449	0.448	0.448
b_3	0.455	0.455	0.455	0.455	0.455	0.455
b_4	0.455	0.455	0.455	0.455	0.455	0.455
b_5	0.456	0.456	0.456	0.456	0.456	0.456
c_2	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_3	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_4	2.74×10^{-3}	2.74×10^{-3}	2.74×10^{-3}	2.75×10^{-3}	2.74×10^{-3}	2.74×10^{-3}
c_5	2.74×10^{-3}	2.74×10^{-3}	2.74×10^{-3}	2.75×10^{-3}	2.74×10^{-3}	2.74×10^{-3}
d_3	-2.34×10^{-5}	-2.27×10^{-5}	-2.28×10^{-5}	-2.41×10^{-5}	-2.26×10^{-5}	-2.27×10^{-5}
d_4	-2.34×10^{-5}	-2.27×10^{-5}	-2.28×10^{-5}	-2.41×10^{-5}	-2.26×10^{-5}	-2.27×10^{-5}
d_5	-2.99×10^{-5}	-2.99×10^{-5}	-2.99×10^{-5}	-2.96×10^{-5}	-2.98×10^{-5}	-2.99×10^{-5}
e_4	1.78×10^{-8}	3.24×10^{-8}	3.20×10^{-8}	-1.43×10^{-8}	3.36×10^{-8}	3.54×10^{-8}
e_5	1.78×10^{-8}	3.24×10^{-8}	3.20×10^{-8}	-1.43×10^{-8}	3.36×10^{-8}	3.54×10^{-8}
g_5	1.39×10^{-8}	1.39×10^{-8}	1.40×10^{-8}	1.31×10^{-8}	1.38×10^{-8}	1.39×10^{-8}
$RMSE_1$	0.517	0.517	0.517	0.517	0.517	0.517
$RMSE_2$	0.030	0.032	0.032	0.030	0.034	0.033
$RMSE_3$	2.03×10^{-3}	2.41×10^{-3}	2.29×10^{-3}	2.24×10^{-3}	2.52×10^{-3}	2.42×10^{-3}
$RMSE_4$	2.00×10^{-3}	2.35×10^{-3}	2.25×10^{-3}	2.29×10^{-3}	2.44×10^{-3}	2.36×10^{-3}
$RMSE_5$	6.59×10^{-4}	7.69×10^{-4}	7.41×10^{-4}	9.10×10^{-4}	7.91×10^{-4}	7.69×10^{-4}
Percent Error 1	7.370	7.254	7.281	7.366	7.209	7.366
Percent Error 2	0.424	0.300	0.329	0.423	0.173	0.423
Percent Error 3	0.020	0.018	0.017	0.029	0.019	0.029
Percent Error 4	0.018	0.016	0.015	0.031	0.017	0.031
Percent Error 5	4.65×10^{-3}	4.90×10^{-3}	4.48×10^{-3}	0.012	5.11×10^{-3}	0.012

Table B.18: Fitting coefficients and errors for the DACCD basis set for the RHF α_{zz} values at zero field.

DACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.440	0.440	0.440	0.440	0.439	0.439
b_2	0.440	0.440	0.440	0.440	0.439	0.439
b_3	0.445	0.445	0.445	0.445	0.445	0.445
b_4	0.445	0.445	0.445	0.445	0.445	0.445
b_5	0.446	0.446	0.446	0.446	0.446	0.446
c_2	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}
c_3	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}	2.71×10^{-3}
c_4	2.69×10^{-3}	2.69×10^{-3}	2.69×10^{-3}	2.70×10^{-3}	2.69×10^{-3}	2.69×10^{-3}
c_5	2.69×10^{-3}	2.69×10^{-3}	2.69×10^{-3}	2.70×10^{-3}	2.69×10^{-3}	2.69×10^{-3}
d_3	-1.90×10^{-5}	-1.83×10^{-5}	-1.84×10^{-5}	-1.96×10^{-5}	-1.82×10^{-5}	-1.82×10^{-5}
d_4	-1.90×10^{-5}	-1.83×10^{-5}	-1.84×10^{-5}	-1.96×10^{-5}	-1.82×10^{-5}	-1.82×10^{-5}
d_5	-2.50×10^{-5}	-2.49×10^{-5}	-2.50×10^{-5}	-2.47×10^{-5}	-2.49×10^{-5}	-2.50×10^{-5}
e_4	4.42×10^{-8}	5.65×10^{-8}	5.62×10^{-8}	1.70×10^{-8}	5.74×10^{-8}	5.90×10^{-8}
e_5	4.42×10^{-8}	5.65×10^{-8}	5.62×10^{-8}	1.70×10^{-8}	5.74×10^{-8}	5.90×10^{-8}
g_5	1.29×10^{-8}	1.29×10^{-8}	1.30×10^{-8}	1.22×10^{-8}	1.28×10^{-8}	1.29×10^{-8}
$RMSE_1$	0.509	0.509	0.509	0.509	0.509	0.509
$RMSE_2$	0.025	0.026	0.026	0.025	0.027	0.027
$RMSE_3$	1.99×10^{-3}	2.38×10^{-3}	2.26×10^{-3}	2.18×10^{-3}	2.51×10^{-3}	2.40×10^{-3}
$RMSE_4$	1.85×10^{-3}	2.17×10^{-3}	2.07×10^{-3}	2.10×10^{-3}	2.25×10^{-3}	2.18×10^{-3}
$RMSE_5$	5.52×10^{-4}	6.47×10^{-4}	6.23×10^{-4}	7.69×10^{-4}	6.66×10^{-4}	6.46×10^{-4}
Percent Error 1	7.115	7.024	7.045	7.111	6.988	7.111
Percent Error 2	0.344	0.242	0.266	0.344	0.207	0.344
Percent Error 3	0.021	0.018	0.017	0.030	0.019	0.030
Percent Error 4	0.016	0.015	0.014	0.028	0.015	0.028
Percent Error 5	3.97×10^{-3}	4.19×10^{-3}	3.83×10^{-3}	0.010	4.41×10^{-3}	0.010

Table B.19: Fitting coefficients and errors for the DACCT basis set for the RHF α_{zz} values at zero field.

DACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.449	0.449	0.449	0.449	0.448	0.448
b_2	0.449	0.449	0.449	0.449	0.448	0.448
b_3	0.456	0.455	0.455	0.456	0.455	0.455
b_4	0.456	0.455	0.455	0.456	0.455	0.455
b_5	0.456	0.456	0.456	0.456	0.456	0.456
c_2	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}
c_3	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}	2.77×10^{-3}
c_4	2.76×10^{-3}	2.76×10^{-3}	2.76×10^{-3}	2.77×10^{-3}	2.76×10^{-3}	2.76×10^{-3}
c_5	2.76×10^{-3}	2.76×10^{-3}	2.76×10^{-3}	2.77×10^{-3}	2.76×10^{-3}	2.76×10^{-3}
d_3	-2.40×10^{-5}	-2.33×10^{-5}	-2.34×10^{-5}	-2.47×10^{-5}	-2.32×10^{-5}	-2.32×10^{-5}
d_4	-2.40×10^{-5}	-2.33×10^{-5}	-2.34×10^{-5}	-2.47×10^{-5}	-2.32×10^{-5}	-2.32×10^{-5}
d_5	-3.08×10^{-5}	-3.08×10^{-5}	-3.08×10^{-5}	-3.05×10^{-5}	-3.07×10^{-5}	-3.08×10^{-5}
e_4	2.27×10^{-8}	3.67×10^{-8}	3.63×10^{-8}	-8.18×10^{-9}	3.78×10^{-8}	3.95×10^{-8}
e_5	2.27×10^{-8}	3.67×10^{-8}	3.63×10^{-8}	-8.18×10^{-9}	3.78×10^{-8}	3.95×10^{-8}
g_5	1.46×10^{-8}	1.46×10^{-8}	1.46×10^{-8}	1.39×10^{-8}	1.44×10^{-8}	1.46×10^{-8}
$RMSE_1$	0.521	0.521	0.521	0.521	0.521	0.521
$RMSE_2$	0.031	0.033	0.032	0.031	0.035	0.034
$RMSE_3$	2.12×10^{-3}	2.52×10^{-3}	2.39×10^{-3}	2.34×10^{-3}	2.64×10^{-3}	2.53×10^{-3}
$RMSE_4$	2.08×10^{-3}	2.44×10^{-3}	2.34×10^{-3}	2.37×10^{-3}	2.54×10^{-3}	2.45×10^{-3}
$RMSE_5$	6.29×10^{-4}	7.35×10^{-4}	7.08×10^{-4}	8.70×10^{-4}	7.56×10^{-4}	7.35×10^{-4}
Percent Error 1	7.415	7.297	7.324	7.411	7.250	7.411
Percent Error 2	0.434	0.307	0.337	0.433	0.260	0.433
Percent Error 3	0.021	0.018	0.017	0.030	0.019	0.030
Percent Error 4	0.018	0.016	0.015	0.031	0.017	0.031
Percent Error 5	4.42×10^{-3}	4.65×10^{-3}	4.26×10^{-3}	0.011	4.85×10^{-3}	0.011

Table B.20: Fitting coefficients and errors for the PC3 basis set for the RHF α_{zz} values at zero field.

PC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.449	0.448	0.448	0.449	0.448	0.448
b_2	0.449	0.448	0.448	0.449	0.448	0.448
b_3	0.455	0.455	0.455	0.455	0.455	0.455
b_4	0.455	0.455	0.455	0.455	0.455	0.455
b_5	0.456	0.456	0.456	0.455	0.456	0.456
c_2	2.72×10^{-3}	2.73×10^{-3}	2.72×10^{-3}	2.72×10^{-3}	2.73×10^{-3}	2.73×10^{-3}
c_3	2.72×10^{-3}	2.73×10^{-3}	2.72×10^{-3}	2.72×10^{-3}	2.73×10^{-3}	2.73×10^{-3}
c_4	2.72×10^{-3}	2.72×10^{-3}	2.71×10^{-3}	2.73×10^{-3}	2.71×10^{-3}	2.71×10^{-3}
c_5	2.72×10^{-3}	2.72×10^{-3}	2.71×10^{-3}	2.73×10^{-3}	2.71×10^{-3}	2.71×10^{-3}
d_3	-2.41×10^{-5}	-2.34×10^{-5}	-2.35×10^{-5}	-2.47×10^{-5}	-2.32×10^{-5}	-2.33×10^{-5}
d_4	-2.41×10^{-5}	-2.34×10^{-5}	-2.35×10^{-5}	-2.47×10^{-5}	-2.32×10^{-5}	-2.33×10^{-5}
d_5	-3.05×10^{-5}	-3.05×10^{-5}	-3.06×10^{-5}	-3.02×10^{-5}	-3.04×10^{-5}	-3.05×10^{-5}
e_4	1.48×10^{-8}	2.90×10^{-8}	2.86×10^{-8}	-1.65×10^{-8}	3.02×10^{-8}	3.19×10^{-8}
e_5	1.48×10^{-8}	2.90×10^{-8}	2.86×10^{-8}	-1.65×10^{-8}	3.02×10^{-8}	3.19×10^{-8}
g_5	1.39×10^{-8}	1.39×10^{-8}	1.40×10^{-8}	1.30×10^{-8}	1.38×10^{-8}	1.39×10^{-8}
$RMSE_1$	0.512	0.512	0.512	0.512	0.512	0.512
$RMSE_2$	0.031	0.033	0.032	0.031	0.035	0.034
$RMSE_3$	2.02×10^{-3}	2.40×10^{-3}	2.28×10^{-3}	2.24×10^{-3}	2.51×10^{-3}	2.41×10^{-3}
$RMSE_4$	2.00×10^{-3}	2.35×10^{-3}	2.25×10^{-3}	2.29×10^{-3}	2.44×10^{-3}	2.36×10^{-3}
$RMSE_5$	6.41×10^{-4}	7.49×10^{-4}	7.21×10^{-4}	8.92×10^{-4}	7.71×10^{-4}	7.48×10^{-4}
Percent Error 1	7.321	7.201	7.229	7.317	7.155	7.317
Percent Error 2	0.435	0.308	0.338	0.435	0.178	0.435
Percent Error 3	0.019	0.018	0.016	0.029	0.019	0.029
Percent Error 4	0.018	0.016	0.015	0.031	0.017	0.031
Percent Error 5	4.60×10^{-3}	4.86×10^{-3}	4.44×10^{-3}	0.012	5.11×10^{-3}	0.012

Table B.21: Fitting coefficients and errors for the APC3 basis set for the RHF α_{zz} values at zero field.

APC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.449	0.448	0.448	0.449	0.448	0.448
b_2	0.449	0.448	0.448	0.449	0.448	0.448
b_3	0.455	0.455	0.455	0.455	0.455	0.455
b_4	0.455	0.455	0.455	0.455	0.455	0.455
b_5	0.455	0.455	0.455	0.455	0.455	0.455
c_2	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_3	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_4	2.74×10^{-3}	2.74×10^{-3}	2.74×10^{-3}	2.75×10^{-3}	2.74×10^{-3}	2.73×10^{-3}
c_5	2.74×10^{-3}	2.74×10^{-3}	2.74×10^{-3}	2.75×10^{-3}	2.74×10^{-3}	2.73×10^{-3}
d_3	-2.32×10^{-5}	-2.25×10^{-5}	-2.26×10^{-5}	-2.39×10^{-5}	-2.24×10^{-5}	-2.25×10^{-5}
d_4	-2.32×10^{-5}	-2.25×10^{-5}	-2.26×10^{-5}	-2.39×10^{-5}	-2.24×10^{-5}	-2.25×10^{-5}
d_5	-2.97×10^{-5}	-2.97×10^{-5}	-2.97×10^{-5}	-2.94×10^{-5}	-2.96×10^{-5}	-2.97×10^{-5}
e_4	3.06×10^{-8}	4.46×10^{-8}	4.42×10^{-8}	-1.21×10^{-10}	4.57×10^{-8}	4.74×10^{-8}
e_5	3.06×10^{-8}	4.46×10^{-8}	4.42×10^{-8}	-1.21×10^{-10}	4.57×10^{-8}	4.74×10^{-8}
g_5	1.38×10^{-8}	1.39×10^{-8}	1.39×10^{-8}	1.31×10^{-8}	1.37×10^{-8}	1.39×10^{-8}
$RMSE_1$	0.517	0.517	0.517	0.517	0.517	0.517
$RMSE_2$	0.030	0.032	0.031	0.030	0.034	0.033
$RMSE_3$	2.05×10^{-3}	2.46×10^{-3}	2.33×10^{-3}	2.27×10^{-3}	2.58×10^{-3}	2.47×10^{-3}
$RMSE_4$	1.99×10^{-3}	2.34×10^{-3}	2.23×10^{-3}	2.27×10^{-3}	2.43×10^{-3}	2.35×10^{-3}
$RMSE_5$	6.28×10^{-4}	7.34×10^{-4}	7.07×10^{-4}	8.71×10^{-4}	7.55×10^{-4}	7.33×10^{-4}
Percent Error 1	7.364	7.249	7.276	7.360	7.204	7.360
Percent Error 2	0.423	0.299	0.328	0.423	0.253	0.423
Percent Error 3	0.021	0.019	0.017	0.030	0.019	0.030
Percent Error 4	0.017	0.016	0.015	0.030	0.017	0.030
Percent Error 5	4.47×10^{-3}	4.72×10^{-3}	4.31×10^{-3}	0.012	4.95×10^{-3}	0.012

Table B.22: Fitting coefficients and errors for the APC4 basis set for the RHF α_{zz} values at zero field.

APC4	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.449	0.448	0.448	0.449	0.448	0.448
b_2	0.449	0.448	0.448	0.449	0.448	0.448
b_3	0.455	0.455	0.455	0.455	0.455	0.455
b_4	0.455	0.455	0.455	0.455	0.455	0.455
b_5	0.455	0.455	0.455	0.455	0.455	0.455
c_2	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_3	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}	2.75×10^{-3}
c_4	2.74×10^{-3}	2.73×10^{-3}	2.73×10^{-3}	2.74×10^{-3}	2.73×10^{-3}	2.73×10^{-3}
c_5	2.74×10^{-3}	2.73×10^{-3}	2.73×10^{-3}	2.74×10^{-3}	2.73×10^{-3}	2.73×10^{-3}
d_3	-2.32×10^{-5}	-2.25×10^{-5}	-2.26×10^{-5}	-2.39×10^{-5}	-2.24×10^{-5}	-2.24×10^{-5}
d_4	-2.32×10^{-5}	-2.25×10^{-5}	-2.26×10^{-5}	-2.39×10^{-5}	-2.24×10^{-5}	-2.24×10^{-5}
d_5	-2.97×10^{-5}	-2.96×10^{-5}	-2.97×10^{-5}	-2.94×10^{-5}	-2.96×10^{-5}	-2.97×10^{-5}
e_4	3.26×10^{-8}	4.65×10^{-8}	4.61×10^{-8}	2.04×10^{-9}	4.75×10^{-8}	4.93×10^{-8}
e_5	3.26×10^{-8}	4.65×10^{-8}	4.61×10^{-8}	2.04×10^{-9}	4.75×10^{-8}	4.93×10^{-8}
g_5	1.39×10^{-8}	1.39×10^{-8}	1.39×10^{-8}	1.31×10^{-8}	1.37×10^{-8}	1.39×10^{-8}
$RMSE_1$	0.517	0.517	0.517	0.517	0.517	0.517
$RMSE_2$	0.030	0.032	0.031	0.030	0.034	0.033
$RMSE_3$	2.06×10^{-3}	2.47×10^{-3}	2.34×10^{-3}	2.28×10^{-3}	2.59×10^{-3}	2.48×10^{-3}
$RMSE_4$	1.99×10^{-3}	2.34×10^{-3}	2.24×10^{-3}	2.27×10^{-3}	2.43×10^{-3}	2.35×10^{-3}
$RMSE_5$	6.24×10^{-4}	7.29×10^{-4}	7.02×10^{-4}	8.65×10^{-4}	7.50×10^{-4}	7.29×10^{-4}
Percent Error 1	7.361	7.246	7.273	7.357	7.201	7.357
Percent Error 2	0.423	0.299	0.328	0.423	0.253	0.423
Percent Error 3	0.021	0.019	0.017	0.031	0.019	0.031
Percent Error 4	0.017	0.016	0.015	0.030	0.017	0.030
Percent Error 5	4.44×10^{-3}	4.59×10^{-3}	4.24×10^{-3}	0.011	4.91×10^{-3}	0.011

B.3 γ_{xxxx} Results

Table B.23: Fitting coefficients and errors for the CCD basis set for the RHF γ_{xxxx} values at zero field.

CCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	0.448	0.442	0.444	0.449	0.440	0.441
b_2	0.448	0.442	0.444	0.449	0.440	0.441
b_3	0.478	0.480	0.480	0.477	0.480	0.480
b_4	0.478	0.480	0.480	0.477	0.480	0.480
b_5	0.471	0.471	0.471	0.470	0.471	0.471
c_2	−0.031	−0.030	−0.030	−0.031	−0.030	−0.030
c_3	−0.031	−0.030	−0.030	−0.031	−0.030	−0.030
c_4	−0.034	−0.034	−0.034	−0.034	−0.034	−0.034
c_5	−0.034	−0.034	−0.034	−0.034	−0.034	−0.034
d_3	-1.19×10^{-4}	-1.27×10^{-4}	-1.26×10^{-4}	-1.11×10^{-4}	-1.29×10^{-4}	-1.28×10^{-4}
d_4	-1.19×10^{-4}	-1.27×10^{-4}	-1.26×10^{-4}	-1.11×10^{-4}	-1.29×10^{-4}	-1.28×10^{-4}
d_5	-3.53×10^{-5}	-3.48×10^{-5}	-3.56×10^{-5}	-2.94×10^{-5}	-3.35×10^{-5}	-3.51×10^{-5}
e_4	9.64×10^{-6}	9.60×10^{-6}	9.60×10^{-6}	9.72×10^{-6}	9.60×10^{-6}	9.59×10^{-6}
e_5	9.64×10^{-6}	9.60×10^{-6}	9.60×10^{-6}	9.72×10^{-6}	9.60×10^{-6}	9.59×10^{-6}
g_5	-1.80×10^{-7}	-1.80×10^{-7}	-1.78×10^{-7}	-1.95×10^{-7}	-1.82×10^{-7}	-1.79×10^{-7}
$RMSE_1$	5.767	5.767	5.767	5.767	5.768	5.767
$RMSE_2$	0.224	0.250	0.240	0.225	0.266	0.256
$RMSE_3$	0.163	0.183	0.175	0.164	0.193	0.186
$RMSE_4$	0.025	0.028	0.027	0.027	0.029	0.028
$RMSE_5$	2.12×10^{-3}	2.51×10^{-3}	2.39×10^{-3}	3.95×10^{-3}	2.70×10^{-3}	2.49×10^{-3}
Percent Error 1	25.756	25.496	25.554	25.768	25.404	25.768
Percent Error 2	2.579	1.269	1.827	2.692	1.419	2.692
Percent Error 3	1.428	0.812	0.760	1.615	0.865	1.615
Percent Error 4	0.121	0.096	0.090	0.190	0.099	0.190
Percent Error 5	0.020	0.022	0.019	0.071	0.025	0.071

Table B.24: Fitting coefficients and errors for the CCT basis set for the RHF γ_{xxxx} values at zero field.

CCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	2.401	2.349	2.361	2.400	2.329	2.338
b_2	2.401	2.349	2.361	2.400	2.329	2.338
b_3	2.717	2.714	2.715	2.719	2.714	2.714
b_4	2.717	2.714	2.715	2.719	2.714	2.714
b_5	2.729	2.729	2.729	2.730	2.729	2.729
c_2	−0.034	−0.034	−0.034	−0.034	−0.034	−0.034
c_3	−0.034	−0.034	−0.034	−0.034	−0.034	−0.034
c_4	−0.037	−0.037	−0.037	−0.036	−0.037	−0.037
c_5	−0.037	−0.037	−0.037	−0.036	−0.037	−0.037
d_3	-1.25×10^{-3}	-1.24×10^{-3}	-1.24×10^{-3}	-1.27×10^{-3}	-1.24×10^{-3}	-1.24×10^{-3}
d_4	-1.25×10^{-3}	-1.24×10^{-3}	-1.24×10^{-3}	-1.27×10^{-3}	-1.24×10^{-3}	-1.24×10^{-3}
d_5	-1.39×10^{-3}	-1.39×10^{-3}	-1.39×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}	-1.39×10^{-3}
e_4	7.27×10^{-6}	7.43×10^{-6}	7.43×10^{-6}	6.91×10^{-6}	7.45×10^{-6}	7.47×10^{-6}
e_5	7.27×10^{-6}	7.43×10^{-6}	7.43×10^{-6}	6.91×10^{-6}	7.45×10^{-6}	7.47×10^{-6}
g_5	3.03×10^{-7}	3.03×10^{-7}	3.02×10^{-7}	3.19×10^{-7}	3.06×10^{-7}	3.03×10^{-7}
$RMSE_1$	6.659	6.688	6.676	6.659	6.714	6.701
$RMSE_2$	1.630	1.745	1.698	1.630	1.843	1.795
$RMSE_3$	0.128	0.147	0.140	0.130	0.156	0.150
$RMSE_4$	0.042	0.049	0.047	0.046	0.050	0.049
$RMSE_5$	8.06×10^{-3}	9.19×10^{-3}	8.89×10^{-3}	0.011	9.44×10^{-3}	9.19×10^{-3}
Percent Error 1	10.886	10.219	10.376	10.875	9.964	10.875
Percent Error 2	5.779	4.031	4.439	5.796	2.927	5.796
Percent Error 3	0.256	0.181	0.168	0.305	0.194	0.305
Percent Error 4	0.069	0.059	0.055	0.114	0.061	0.114
Percent Error 5	0.027	0.025	0.023	0.073	0.026	0.073

Table B.25: Fitting coefficients and errors for the CCQ basis set for the RHF γ_{xxxx} values at zero field.

CCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	4.768	4.708	4.722	4.768	4.685	4.696
b_2	4.768	4.708	4.722	4.768	4.685	4.696
b_3	5.121	5.121	5.121	5.122	5.121	5.121
b_4	5.121	5.121	5.121	5.122	5.121	5.121
b_5	5.123	5.123	5.123	5.124	5.123	5.123
c_2	-0.012	-0.012	-0.012	-0.012	-0.012	-0.012
c_3	-0.012	-0.012	-0.012	-0.012	-0.012	-0.012
c_4	-0.014	-0.014	-0.014	-0.014	-0.014	-0.014
c_5	-0.014	-0.014	-0.014	-0.014	-0.014	-0.014
d_3	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}
d_4	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}	-1.40×10^{-3}
d_5	-1.43×10^{-3}	-1.43×10^{-3}	-1.43×10^{-3}	-1.43×10^{-3}	-1.43×10^{-3}	-1.43×10^{-3}
e_4	7.15×10^{-6}	7.14×10^{-6}	7.14×10^{-6}	7.18×10^{-6}	7.14×10^{-6}	7.14×10^{-6}
e_5	7.15×10^{-6}	7.14×10^{-6}	7.14×10^{-6}	7.18×10^{-6}	7.14×10^{-6}	7.14×10^{-6}
g_5	5.37×10^{-8}	5.32×10^{-8}	5.27×10^{-8}	6.46×10^{-8}	5.45×10^{-8}	5.27×10^{-8}
$RMSE_1$	2.886	2.973	2.937	2.886	3.049	3.011
$RMSE_2$	1.822	1.957	1.902	1.822	2.071	2.016
$RMSE_3$	0.120	0.134	0.129	0.120	0.142	0.137
$RMSE_4$	7.41×10^{-3}	8.39×10^{-3}	8.10×10^{-3}	7.98×10^{-3}	8.67×10^{-3}	8.44×10^{-3}
$RMSE_5$	1.18×10^{-3}	1.30×10^{-3}	1.26×10^{-3}	2.30×10^{-3}	1.37×10^{-3}	1.29×10^{-3}
Percent Error 1	2.822	2.428	2.521	2.819	2.278	2.819
Percent Error 2	3.596	2.511	2.765	3.608	1.876	3.608
Percent Error 3	0.099	0.078	0.074	0.109	0.082	0.109
Percent Error 4	0.014	0.010	9.35×10^{-3}	0.022	0.010	0.022
Percent Error 5	8.94×10^{-4}	9.90×10^{-4}	8.83×10^{-4}	3.66×10^{-3}	1.13×10^{-3}	3.66×10^{-3}

Table B.26: Fitting coefficients and errors for the ACCD basis set for the RHF γ_{xxxx} values at zero field.

ACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	12.108	12.026	12.045	12.108	11.994	12.009
b_2	12.108	12.026	12.045	12.108	11.994	12.009
b_3	12.599	12.597	12.597	12.601	12.596	12.596
b_4	12.599	12.597	12.597	12.601	12.596	12.596
b_5	12.611	12.611	12.610	12.611	12.611	12.611
c_2	0.096	0.096	0.096	0.096	0.096	0.096
c_3	0.096	0.096	0.096	0.096	0.096	0.096
c_4	0.096	0.096	0.096	0.096	0.096	0.096
c_5	0.096	0.096	0.096	0.096	0.096	0.096
d_3	-1.95×10^{-3}	-1.93×10^{-3}	-1.94×10^{-3}	-1.96×10^{-3}	-1.93×10^{-3}	-1.93×10^{-3}
d_4	-1.95×10^{-3}	-1.93×10^{-3}	-1.94×10^{-3}	-1.96×10^{-3}	-1.93×10^{-3}	-1.93×10^{-3}
d_5	-2.08×10^{-3}	-2.08×10^{-3}	-2.08×10^{-3}	-2.09×10^{-3}	-2.08×10^{-3}	-2.08×10^{-3}
e_4	-8.91×10^{-7}	-1.00×10^{-6}	-1.00×10^{-6}	-6.46×10^{-7}	-1.02×10^{-6}	-1.03×10^{-6}
e_5	-8.91×10^{-7}	-1.00×10^{-6}	-9.98×10^{-7}	-6.46×10^{-7}	-1.02×10^{-6}	-1.03×10^{-6}
g_5	2.81×10^{-7}	2.81×10^{-7}	2.78×10^{-7}	3.12×10^{-7}	2.86×10^{-7}	2.79×10^{-7}
$RMSE_1$	18.156	18.183	18.172	18.156	18.206	18.195
$RMSE_2$	2.527	2.709	2.635	2.527	2.864	2.789
$RMSE_3$	0.041	0.048	0.046	0.044	0.050	0.048
$RMSE_4$	0.039	0.044	0.043	0.042	0.046	0.044
$RMSE_5$	5.85×10^{-3}	6.76×10^{-3}	6.50×10^{-3}	9.44×10^{-3}	7.10×10^{-3}	6.74×10^{-3}
Percent Error 1	20.372	19.608	19.788	20.364	19.316	20.364
Percent Error 2	0.833	0.590	0.647	0.831	0.754	0.831
Percent Error 3	0.060	0.042	0.039	0.083	0.043	0.083
Percent Error 4	0.044	0.032	0.030	0.070	0.034	0.070
Percent Error 5	2.30×10^{-3}	2.59×10^{-3}	2.30×10^{-3}	7.41×10^{-3}	2.88×10^{-3}	7.41×10^{-3}

Table B.27: Fitting coefficients and errors for the ACCT basis set for the RHF γ_{xxxx} values at zero field.

ACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	14.742	14.667	14.685	14.742	14.639	14.652
b_2	14.742	14.667	14.685	14.742	14.639	14.652
b_3	15.175	15.176	15.176	15.174	15.176	15.176
b_4	15.175	15.176	15.176	15.174	15.176	15.176
b_5	15.169	15.169	15.169	15.169	15.169	15.169
c_2	0.121	0.121	0.121	0.122	0.121	0.121
c_3	0.121	0.121	0.121	0.122	0.121	0.121
c_4	0.125	0.125	0.125	0.125	0.125	0.125
c_5	0.125	0.125	0.125	0.125	0.125	0.125
d_3	-1.72×10^{-3}	-1.73×10^{-3}	-1.72×10^{-3}	-1.71×10^{-3}	-1.73×10^{-3}	-1.73×10^{-3}
d_4	-1.72×10^{-3}	-1.73×10^{-3}	-1.72×10^{-3}	-1.71×10^{-3}	-1.73×10^{-3}	-1.73×10^{-3}
d_5	-1.65×10^{-3}	-1.65×10^{-3}	-1.65×10^{-3}	-1.65×10^{-3}	-1.65×10^{-3}	-1.65×10^{-3}
e_4	-1.13×10^{-5}	-1.11×10^{-5}	-1.12×10^{-5}	-1.16×10^{-5}	-1.11×10^{-5}	-1.11×10^{-5}
e_5	-1.13×10^{-5}	-1.11×10^{-5}	-1.12×10^{-5}	-1.16×10^{-5}	-1.11×10^{-5}	-1.11×10^{-5}
g_5	-1.48×10^{-7}	-1.49×10^{-7}	-1.49×10^{-7}	-1.47×10^{-7}	-1.48×10^{-7}	-1.49×10^{-7}
$RMSE_1$	22.914	22.932	22.924	22.914	22.947	22.939
$RMSE_2$	2.237	2.409	2.339	2.237	2.553	2.482
$RMSE_3$	0.190	0.211	0.203	0.190	0.223	0.215
$RMSE_4$	0.021	0.025	0.024	0.024	0.026	0.025
$RMSE_5$	6.48×10^{-3}	7.51×10^{-3}	7.25×10^{-3}	8.82×10^{-3}	7.71×10^{-3}	7.52×10^{-3}
Percent Error 1	18.191	17.678	17.799	18.191	17.484	18.191
Percent Error 2	0.640	0.445	0.490	0.643	0.551	0.643
Percent Error 3	0.056	0.047	0.044	0.062	0.049	0.062
Percent Error 4	0.021	0.016	0.015	0.036	0.017	0.036
Percent Error 5	1.62×10^{-3}	1.70×10^{-3}	1.58×10^{-3}	0.011	1.76×10^{-3}	0.011

Table B.28: Fitting coefficients and errors for the ACCQ basis set for the RHF γ_{xxxx} values at zero field.

ACCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	17.161	17.074	17.095	17.161	17.041	17.057
b_2	17.161	17.074	17.095	17.161	17.041	17.057
b_3	17.671	17.670	17.670	17.671	17.670	17.670
b_4	17.671	17.670	17.670	17.671	17.670	17.670
b_5	17.674	17.674	17.674	17.675	17.674	17.674
c_2	0.145	0.144	0.144	0.145	0.144	0.144
c_3	0.145	0.144	0.144	0.145	0.144	0.144
c_4	0.149	0.149	0.149	0.150	0.149	0.149
c_5	0.149	0.149	0.149	0.150	0.149	0.149
d_3	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}
d_4	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}	-2.02×10^{-3}
d_5	-2.06×10^{-3}	-2.06×10^{-3}	-2.05×10^{-3}	-2.07×10^{-3}	-2.06×10^{-3}	-2.06×10^{-3}
e_4	-1.66×10^{-5}	-1.65×10^{-5}	-1.65×10^{-5}	-1.69×10^{-5}	-1.64×10^{-5}	-1.64×10^{-5}
e_5	-1.66×10^{-5}	-1.65×10^{-5}	-1.65×10^{-5}	-1.69×10^{-5}	-1.64×10^{-5}	-1.64×10^{-5}
g_5	7.33×10^{-8}	7.26×10^{-8}	6.97×10^{-8}	1.11×10^{-7}	7.82×10^{-8}	7.09×10^{-8}
$RMSE_1$	27.259	27.278	27.270	27.259	27.296	27.287
$RMSE_2$	2.637	2.834	2.754	2.637	3.000	2.919
$RMSE_3$	0.277	0.310	0.298	0.278	0.327	0.316
$RMSE_4$	0.012	0.013	0.013	0.014	0.014	0.013
$RMSE_5$	6.93×10^{-3}	8.14×10^{-3}	7.80×10^{-3}	0.012	8.54×10^{-3}	8.10×10^{-3}
Percent Error 1	17.810	17.319	17.434	17.807	17.133	17.807
Percent Error 2	0.644	0.446	0.493	0.648	0.557	0.648
Percent Error 3	0.189	0.116	0.110	0.204	0.123	0.204
Percent Error 4	3.07×10^{-3}	2.72×10^{-3}	2.61×10^{-3}	5.58×10^{-3}	2.82×10^{-3}	5.58×10^{-3}
Percent Error 5	5.52×10^{-3}	5.72×10^{-3}	5.09×10^{-3}	0.018	6.34×10^{-3}	0.018

Table B.29: Fitting coefficients and errors for the DACCD basis set for the RHF γ_{xxxx} values at zero field.

DACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	18.409	18.336	18.353	18.409	18.308	18.320
b_2	18.409	18.336	18.353	18.409	18.308	18.321
b_3	18.835	18.836	18.836	18.835	18.836	18.836
b_4	18.835	18.836	18.836	18.835	18.836	18.836
b_5	18.835	18.835	18.835	18.835	18.835	18.835
c_2	0.178	0.177	0.177	0.178	0.177	0.177
c_3	0.178	0.177	0.177	0.178	0.177	0.177
c_4	0.185	0.184	0.184	0.185	0.185	0.184
c_5	0.185	0.184	0.184	0.185	0.185	0.184
d_3	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}	-1.70×10^{-3}	-1.70×10^{-3}
d_4	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}	-1.70×10^{-3}	-1.70×10^{-3}
d_5	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}	-1.69×10^{-3}
e_4	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}
e_5	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}	-2.23×10^{-5}
g_5	-1.18×10^{-8}	-1.19×10^{-8}	-1.29×10^{-8}	2.13×10^{-9}	-1.00×10^{-8}	-1.24×10^{-8}
$RMSE_1$	33.461	33.473	33.468	33.461	33.483	33.478
$RMSE_2$	2.228	2.399	2.330	2.229	2.540	2.470
$RMSE_3$	0.372	0.418	0.401	0.373	0.442	0.427
$RMSE_4$	2.00×10^{-3}	2.61×10^{-3}	2.44×10^{-3}	2.58×10^{-3}	2.74×10^{-3}	2.62×10^{-3}
$RMSE_5$	1.18×10^{-3}	1.40×10^{-3}	1.32×10^{-3}	2.85×10^{-3}	1.56×10^{-3}	1.37×10^{-3}
Percent Error 1	19.322	18.946	19.035	19.321	18.803	19.321
Percent Error 2	0.531	0.363	0.402	0.536	0.460	0.536
Percent Error 3	0.081	0.070	0.066	0.087	0.074	0.087
Percent Error 4	1.74×10^{-3}	1.59×10^{-3}	1.41×10^{-3}	3.19×10^{-3}	1.69×10^{-3}	3.19×10^{-3}
Percent Error 5	7.89×10^{-4}	9.73×10^{-4}	8.47×10^{-4}	3.45×10^{-3}	1.13×10^{-3}	3.45×10^{-3}

Table B.30: Fitting coefficients and errors for the DACCT basis set for the RHF γ_{xxxx} values at zero field.

DACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	20.557	20.463	20.485	20.557	20.427	20.444
b_2	20.557	20.463	20.485	20.557	20.427	20.444
b_3	21.108	21.107	21.107	21.108	21.107	21.107
b_4	21.108	21.107	21.107	21.108	21.107	21.107
b_5	21.109	21.109	21.109	21.109	21.109	21.109
c_2	0.181	0.180	0.180	0.181	0.180	0.180
c_3	0.181	0.180	0.180	0.181	0.180	0.180
c_4	0.187	0.187	0.187	0.187	0.187	0.187
c_5	0.187	0.187	0.187	0.187	0.187	0.187
d_3	-2.19×10^{-3}	-2.18×10^{-3}	-2.18×10^{-3}	-2.19×10^{-3}	-2.18×10^{-3}	-2.18×10^{-3}
d_4	-2.19×10^{-3}	-2.18×10^{-3}	-2.18×10^{-3}	-2.19×10^{-3}	-2.18×10^{-3}	-2.18×10^{-3}
d_5	-2.20×10^{-3}	-2.20×10^{-3}	-2.20×10^{-3}	-2.20×10^{-3}	-2.20×10^{-3}	-2.20×10^{-3}
e_4	-1.94×10^{-5}	-1.93×10^{-5}	-1.93×10^{-5}	-1.97×10^{-5}	-1.93×10^{-5}	-1.93×10^{-5}
e_5	-1.94×10^{-5}	-1.93×10^{-5}	-1.93×10^{-5}	-1.97×10^{-5}	-1.93×10^{-5}	-1.93×10^{-5}
g_5	3.26×10^{-8}	3.26×10^{-8}	3.28×10^{-8}	3.08×10^{-8}	3.23×10^{-8}	3.26×10^{-8}
$RMSE_1$	34.095	34.113	34.106	34.095	34.130	34.121
$RMSE_2$	2.853	3.068	2.980	2.853	3.247	3.159
$RMSE_3$	0.324	0.363	0.349	0.326	0.384	0.370
$RMSE_4$	7.60×10^{-3}	8.79×10^{-3}	8.46×10^{-3}	9.58×10^{-3}	9.06×10^{-3}	8.81×10^{-3}
$RMSE_5$	6.17×10^{-3}	7.08×10^{-3}	6.84×10^{-3}	8.21×10^{-3}	7.26×10^{-3}	7.08×10^{-3}
Percent Error 1	18.910	18.454	18.562	18.908	18.281	18.908
Percent Error 2	0.592	0.409	0.452	0.596	0.514	0.596
Percent Error 3	0.189	0.114	0.108	0.204	0.121	0.204
Percent Error 4	1.91×10^{-3}	1.86×10^{-3}	1.73×10^{-3}	3.78×10^{-3}	1.93×10^{-3}	3.78×10^{-3}
Percent Error 5	1.07×10^{-3}	1.12×10^{-3}	1.05×10^{-3}	2.55×10^{-3}	1.17×10^{-3}	2.55×10^{-3}

Table B.31: Fitting coefficients and errors for the PC3 basis set for the RHF γ_{xxxx} values at zero field.

PC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	9.902	9.833	9.849	9.902	9.807	9.819
b_2	9.902	9.833	9.849	9.902	9.807	9.819
b_3	10.299	10.300	10.300	10.297	10.301	10.301
b_4	10.299	10.300	10.300	10.297	10.301	10.301
b_5	10.290	10.289	10.290	10.288	10.289	10.289
c_2	0.064	0.064	0.064	0.064	0.064	0.064
c_3	0.064	0.064	0.064	0.064	0.064	0.064
c_4	0.066	0.066	0.066	0.066	0.066	0.066
c_5	0.066	0.066	0.066	0.066	0.066	0.066
d_3	-1.58×10^{-3}	-1.58×10^{-3}	-1.58×10^{-3}	-1.57×10^{-3}	-1.59×10^{-3}	-1.59×10^{-3}
d_4	-1.58×10^{-3}	-1.58×10^{-3}	-1.58×10^{-3}	-1.57×10^{-3}	-1.59×10^{-3}	-1.59×10^{-3}
d_5	-1.47×10^{-3}	-1.47×10^{-3}	-1.47×10^{-3}	-1.46×10^{-3}	-1.47×10^{-3}	-1.47×10^{-3}
e_4	-7.35×10^{-6}	-7.11×10^{-6}	-7.13×10^{-6}	-7.85×10^{-6}	-7.07×10^{-6}	-7.06×10^{-6}
e_5	-7.35×10^{-6}	-7.11×10^{-6}	-7.13×10^{-6}	-7.85×10^{-6}	-7.07×10^{-6}	-7.06×10^{-6}
g_5	-2.20×10^{-7}	-2.20×10^{-7}	-2.15×10^{-7}	-2.68×10^{-7}	-2.28×10^{-7}	-2.18×10^{-7}
$RMSE_1$	12.208	12.236	12.224	12.208	12.260	12.248
$RMSE_2$	2.048	2.206	2.141	2.048	2.339	2.273
$RMSE_3$	0.127	0.140	0.135	0.128	0.147	0.142
$RMSE_4$	0.033	0.037	0.036	0.036	0.038	0.037
$RMSE_5$	0.013	0.015	0.015	0.019	0.015	0.015
Percent Error 1	14.132	13.482	13.636	14.132	13.237	14.132
Percent Error 2	0.835	0.583	0.642	0.837	0.723	0.837
Percent Error 3	0.056	0.045	0.043	0.063	0.047	0.063
Percent Error 4	0.040	0.030	0.029	0.067	0.031	0.067
Percent Error 5	5.13×10^{-3}	5.51×10^{-3}	4.96×10^{-3}	0.015	6.04×10^{-3}	0.015

Table B.32: Fitting coefficients and errors for the APC3 basis set for the RHF γ_{xxxx} values at zero field.

APC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	21.117	21.025	21.047	21.116	20.990	21.006
b_2	21.117	21.025	21.047	21.116	20.990	21.006
b_3	21.651	21.652	21.652	21.651	21.652	21.652
b_4	21.651	21.652	21.652	21.651	21.652	21.652
b_5	21.650	21.650	21.650	21.650	21.650	21.650
c_2	0.192	0.191	0.191	0.192	0.191	0.191
c_3	0.192	0.191	0.191	0.192	0.191	0.191
c_4	0.197	0.197	0.197	0.197	0.197	0.197
c_5	0.197	0.197	0.197	0.197	0.197	0.197
d_3	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}
d_4	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}	-2.12×10^{-3}
d_5	-2.11×10^{-3}	-2.11×10^{-3}	-2.11×10^{-3}	-2.10×10^{-3}	-2.11×10^{-3}	-2.11×10^{-3}
e_4	-1.72×10^{-5}	-1.72×10^{-5}	-1.72×10^{-5}	-1.71×10^{-5}	-1.72×10^{-5}	-1.72×10^{-5}
e_5	-1.72×10^{-5}	-1.72×10^{-5}	-1.72×10^{-5}	-1.71×10^{-5}	-1.72×10^{-5}	-1.72×10^{-5}
g_5	-2.50×10^{-8}	-2.48×10^{-8}	-2.33×10^{-8}	-4.30×10^{-8}	-2.76×10^{-8}	-2.42×10^{-8}
$RMSE_1$	36.116	36.132	36.126	36.116	36.147	36.140
$RMSE_2$	2.768	2.977	2.892	2.768	3.153	3.066
$RMSE_3$	0.287	0.323	0.309	0.288	0.342	0.329
$RMSE_4$	3.90×10^{-3}	4.15×10^{-3}	4.07×10^{-3}	4.17×10^{-3}	4.24×10^{-3}	4.16×10^{-3}
$RMSE_5$	1.89×10^{-3}	2.25×10^{-3}	2.13×10^{-3}	4.02×10^{-3}	2.46×10^{-3}	2.22×10^{-3}
Percent Error 1	19.692	19.253	19.356	19.690	19.087	19.690
Percent Error 2	0.559	0.387	0.427	0.563	0.485	0.563
Percent Error 3	0.056	0.048	0.046	0.060	0.051	0.060
Percent Error 4	6.57×10^{-4}	5.89×10^{-4}	7.29×10^{-4}	1.11×10^{-3}	6.02×10^{-4}	1.11×10^{-3}
Percent Error 5	1.33×10^{-3}	1.54×10^{-3}	1.34×10^{-3}	5.16×10^{-3}	1.77×10^{-3}	5.16×10^{-3}

Table B.33: Fitting coefficients and errors for the APC4 basis set for the RHF γ_{xxxx} values at zero field.

APC4	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	21.022	20.931	20.953	21.021	20.897	20.913
b_2	21.022	20.931	20.953	21.021	20.897	20.913
b_3	21.548	21.549	21.548	21.548	21.550	21.549
b_4	21.548	21.549	21.548	21.548	21.550	21.549
b_5	21.548	21.548	21.548	21.550	21.548	21.548
c_2	0.188	0.188	0.188	0.188	0.187	0.187
c_3	0.188	0.188	0.188	0.188	0.187	0.187
c_4	0.194	0.194	0.194	0.194	0.194	0.194
c_5	0.194	0.194	0.194	0.194	0.194	0.194
d_3	-2.09×10^{-3}	-2.09×10^{-3}	-2.09×10^{-3}	-2.09×10^{-3}	-2.10×10^{-3}	-2.09×10^{-3}
d_4	-2.09×10^{-3}	-2.09×10^{-3}	-2.09×10^{-3}	-2.09×10^{-3}	-2.10×10^{-3}	-2.09×10^{-3}
d_5	-2.09×10^{-3}	-2.08×10^{-3}	-2.09×10^{-3}	-2.12×10^{-3}	-2.08×10^{-3}	-2.08×10^{-3}
e_4	-1.86×10^{-5}	-1.87×10^{-5}	-1.86×10^{-5}	-1.83×10^{-5}	-1.89×10^{-5}	-1.88×10^{-5}
e_5	-1.86×10^{-5}	-1.87×10^{-5}	-1.86×10^{-5}	-1.83×10^{-5}	-1.89×10^{-5}	-1.88×10^{-5}
g_5	-5.87×10^{-9}	-2.04×10^{-8}	-4.88×10^{-9}	7.28×10^{-8}	-2.58×10^{-8}	-2.21×10^{-8}
$RMSE_1$	35.470	35.486	35.479	35.470	35.501	35.493
$RMSE_2$	2.731	2.937	2.854	2.731	3.109	3.024
$RMSE_3$	0.311	0.349	0.335	0.312	0.369	0.356
$RMSE_4$	8.89×10^{-3}	9.65×10^{-3}	9.17×10^{-3}	0.011	0.013	0.010
$RMSE_5$	8.85×10^{-3}	9.78×10^{-3}	9.10×10^{-3}	0.017	0.014	0.010
Percent Error 1	19.238	18.807	18.908	19.235	18.645	19.235
Percent Error 2	0.557	0.385	0.425	0.561	0.481	0.561
Percent Error 3	0.061	0.052	0.049	0.065	0.055	0.065
Percent Error 4	2.86×10^{-3}	3.56×10^{-3}	2.83×10^{-3}	3.59×10^{-3}	4.83×10^{-3}	3.59×10^{-3}
Percent Error 5	2.92×10^{-3}	3.78×10^{-3}	2.76×10^{-3}	4.52×10^{-3}	5.09×10^{-3}	4.52×10^{-3}

B.4 γ_{zzzz} Results

Table B.34: Fitting coefficients and errors for the CCD basis set for the RHF γ_{zzzz} values at zero field.

CCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	-5.468	-5.221	-5.280	-5.470	-5.130	-5.173
b_2	-5.468	-5.221	-5.280	-5.470	-5.130	-5.173
b_3	-6.837	-6.851	-6.850	-6.820	-6.855	-6.855
b_4	-6.837	-6.851	-6.850	-6.820	-6.855	-6.855
b_5	-6.759	-6.759	-6.759	-6.758	-6.758	-6.759
c_2	-3.67×10^{-3}	4.03×10^{-3}	2.34×10^{-3}	-4.98×10^{-3}	5.96×10^{-3}	4.72×10^{-3}
c_3	-3.67×10^{-3}	4.03×10^{-3}	2.34×10^{-3}	-4.98×10^{-3}	5.96×10^{-3}	4.72×10^{-3}
c_4	-0.054	-0.054	-0.054	-0.054	-0.054	-0.054
c_5	-0.054	-0.054	-0.054	-0.054	-0.054	-0.054
d_3	5.44×10^{-3}	5.53×10^{-3}	5.51×10^{-3}	5.35×10^{-3}	5.54×10^{-3}	5.53×10^{-3}
d_4	5.44×10^{-3}	5.53×10^{-3}	5.51×10^{-3}	5.35×10^{-3}	5.54×10^{-3}	5.53×10^{-3}
d_5	4.57×10^{-3}	4.56×10^{-3}	4.57×10^{-3}	4.55×10^{-3}	4.56×10^{-3}	4.57×10^{-3}
e_4	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}
e_5	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}	1.69×10^{-4}
g_5	1.87×10^{-6}	1.87×10^{-6}	1.86×10^{-6}	1.91×10^{-6}	1.88×10^{-6}	1.87×10^{-6}
$RMSE_1$	7.627	8.166	7.945	7.627	8.613	8.388
$RMSE_2$	7.596	8.264	7.995	7.600	8.774	8.507
$RMSE_3$	2.827	3.179	3.046	2.840	3.359	3.240
$RMSE_4$	0.255	0.295	0.283	0.279	0.306	0.297
$RMSE_5$	8.03×10^{-3}	9.91×10^{-3}	9.38×10^{-3}	0.014	0.011	9.84×10^{-3}
Percent Error 1	10.181	7.898	8.439	10.204	7.795	10.204
Percent Error 2	10.860	7.151	8.006	11.125	7.959	11.125
Percent Error 3	3.400	2.461	2.354	3.787	2.634	3.787
Percent Error 4	1.944	1.128	1.063	3.050	1.270	3.050
Percent Error 5	0.012	0.014	0.012	0.038	0.015	0.038

Table B.35: Fitting coefficients and errors for the CCT basis set for the RHF γ_{zzzz} values at zero field.

CCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	-5.013	-4.699	-4.774	-5.018	-4.583	-4.638
b_2	-5.013	-4.699	-4.774	-5.018	-4.583	-4.638
b_3	-6.722	-6.748	-6.745	-6.692	-6.755	-6.753
b_4	-6.722	-6.748	-6.745	-6.692	-6.755	-6.753
b_5	-6.584	-6.583	-6.584	-6.581	-6.583	-6.584
c_2	0.027	0.038	0.036	0.025	0.041	0.039
c_3	0.027	0.038	0.036	0.025	0.041	0.039
c_4	-0.045	-0.045	-0.045	-0.045	-0.045	-0.045
c_5	-0.045	-0.045	-0.045	-0.045	-0.045	-0.045
d_3	6.79×10^{-3}	6.94×10^{-3}	6.92×10^{-3}	6.64×10^{-3}	6.98×10^{-3}	6.96×10^{-3}
d_4	6.79×10^{-3}	6.94×10^{-3}	6.92×10^{-3}	6.64×10^{-3}	6.98×10^{-3}	6.96×10^{-3}
d_5	5.25×10^{-3}	5.25×10^{-3}	5.25×10^{-3}	5.20×10^{-3}	5.24×10^{-3}	5.25×10^{-3}
e_4	2.41×10^{-4}	2.40×10^{-4}	2.40×10^{-4}	2.41×10^{-4}	2.40×10^{-4}	2.40×10^{-4}
e_5	2.41×10^{-4}	2.40×10^{-4}	2.40×10^{-4}	2.41×10^{-4}	2.40×10^{-4}	2.40×10^{-4}
g_5	3.31×10^{-6}	3.30×10^{-6}	3.29×10^{-6}	3.43×10^{-6}	3.32×10^{-6}	3.30×10^{-6}
$RMSE_1$	10.939	11.551	11.299	10.939	12.063	11.802
$RMSE_2$	9.686	10.575	10.218	9.692	11.239	10.886
$RMSE_3$	4.041	4.543	4.354	4.061	4.801	4.631
$RMSE_4$	0.451	0.521	0.500	0.494	0.541	0.524
$RMSE_5$	0.016	0.019	0.018	0.031	0.021	0.019
Percent Error 1	37.310	31.684	33.021	37.399	29.602	37.399
Percent Error 2	27.598	18.036	20.236	28.352	17.416	28.352
Percent Error 3	9.558	5.932	5.636	10.718	6.340	10.718
Percent Error 4	2.242	2.740	2.581	3.519	2.525	3.519
Percent Error 5	0.045	0.049	0.044	0.158	0.055	0.158

Table B.36: Fitting coefficients and errors for the CCQ basis set for the RHF γ_{zzzz} values at zero field.

CCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	-3.202	-2.857	-2.939	-3.211	-2.730	-2.792
b_2	-3.202	-2.857	-2.939	-3.211	-2.730	-2.792
b_3	-5.021	-5.064	-5.059	-4.972	-5.076	-5.073
b_4	-5.021	-5.064	-5.059	-4.972	-5.076	-5.073
b_5	-4.794	-4.793	-4.794	-4.788	-4.791	-4.793
c_2	0.081	0.092	0.090	0.079	0.095	0.093
c_3	0.081	0.092	0.090	0.079	0.095	0.093
c_4	0.010	0.010	0.010	0.011	0.010	0.010
c_5	0.010	0.010	0.010	0.011	0.010	0.010
d_3	7.22×10^{-3}	7.48×10^{-3}	7.44×10^{-3}	6.99×10^{-3}	7.53×10^{-3}	7.51×10^{-3}
d_4	7.22×10^{-3}	7.48×10^{-3}	7.44×10^{-3}	6.99×10^{-3}	7.53×10^{-3}	7.51×10^{-3}
d_5	4.69×10^{-3}	4.68×10^{-3}	4.69×10^{-3}	4.59×10^{-3}	4.66×10^{-3}	4.68×10^{-3}
e_4	2.36×10^{-4}	2.37×10^{-4}	2.37×10^{-4}	2.33×10^{-4}	2.37×10^{-4}	2.37×10^{-4}
e_5	2.36×10^{-4}	2.37×10^{-4}	2.37×10^{-4}	2.33×10^{-4}	2.37×10^{-4}	2.37×10^{-4}
g_5	5.45×10^{-6}	5.45×10^{-6}	5.43×10^{-6}	5.70×10^{-6}	5.49×10^{-6}	5.44×10^{-6}
$RMSE_1$	18.310	18.760	18.573	18.310	19.142	18.943
$RMSE_2$	10.188	11.170	10.774	10.195	11.901	11.509
$RMSE_3$	4.004	4.527	4.332	4.034	4.790	4.614
$RMSE_4$	0.746	0.861	0.826	0.817	0.893	0.865
$RMSE_5$	0.068	0.079	0.076	0.101	0.082	0.079
Percent Error 1	45.001	40.224	41.362	45.121	38.475	45.121
Percent Error 2	22.595	14.772	16.580	23.259	22.134	23.259
Percent Error 3	7.797	7.694	7.200	8.961	8.191	8.961
Percent Error 4	1.246	1.373	1.294	1.990	1.348	1.990
Percent Error 5	0.078	0.085	0.075	0.231	0.093	0.231

Table B.37: Fitting coefficients and errors for the ACCD basis set for the RHF γ_{zzzz} values at zero field.

ACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	8.740	9.188	9.082	8.731	9.353	9.274
b_2	8.740	9.188	9.082	8.731	9.353	9.274
b_3	6.335	6.290	6.295	6.387	6.278	6.281
b_4	6.335	6.290	6.295	6.387	6.278	6.281
b_5	6.566	6.566	6.566	6.565	6.566	6.566
c_2	0.258	0.271	0.268	0.255	0.275	0.273
c_3	0.258	0.271	0.268	0.255	0.275	0.273
c_4	0.171	0.170	0.170	0.172	0.170	0.170
c_5	0.171	0.170	0.170	0.172	0.170	0.170
d_3	9.55×10^{-3}	9.82×10^{-3}	9.78×10^{-3}	9.30×10^{-3}	9.88×10^{-3}	9.85×10^{-3}
d_4	9.55×10^{-3}	9.82×10^{-3}	9.78×10^{-3}	9.30×10^{-3}	9.88×10^{-3}	9.85×10^{-3}
d_5	6.97×10^{-3}	6.97×10^{-3}	6.97×10^{-3}	6.98×10^{-3}	6.98×10^{-3}	6.97×10^{-3}
e_4	2.91×10^{-4}	2.94×10^{-4}	2.93×10^{-4}	2.86×10^{-4}	2.94×10^{-4}	2.94×10^{-4}
e_5	2.91×10^{-4}	2.94×10^{-4}	2.93×10^{-4}	2.86×10^{-4}	2.94×10^{-4}	2.94×10^{-4}
g_5	5.55×10^{-6}	5.55×10^{-6}	5.55×10^{-6}	5.52×10^{-6}	5.54×10^{-6}	5.55×10^{-6}
$RMSE_1$	50.198	50.477	50.360	50.198	50.719	50.593
$RMSE_2$	13.329	14.575	14.073	13.338	15.513	15.014
$RMSE_3$	4.916	5.569	5.324	4.951	5.897	5.676
$RMSE_4$	0.765	0.890	0.853	0.848	0.925	0.895
$RMSE_5$	0.114	0.132	0.127	0.155	0.136	0.132
Percent Error 1	16.721	15.688	15.934	16.742	15.308	16.742
Percent Error 2	4.840	3.174	3.559	4.977	4.315	4.977
Percent Error 3	1.577	1.363	1.274	1.804	1.455	1.804
Percent Error 4	0.229	0.218	0.201	0.379	0.226	0.379
Percent Error 5	0.029	0.032	0.030	0.069	0.034	0.069

Table B.38: Fitting coefficients and errors for the ACCT basis set for the RHF γ_{zzzz} values at zero field.

ACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	10.138	10.573	10.469	10.128	10.733	10.656
b_2	10.138	10.573	10.469	10.128	10.733	10.656
b_3	7.812	7.767	7.772	7.866	7.754	7.757
b_4	7.812	7.767	7.772	7.866	7.754	7.757
b_5	8.050	8.050	8.050	8.051	8.050	8.050
c_2	0.215	0.230	0.227	0.212	0.234	0.231
c_3	0.215	0.230	0.227	0.212	0.234	0.231
c_4	0.121	0.121	0.121	0.122	0.121	0.120
c_5	0.121	0.121	0.121	0.122	0.121	0.120
d_3	9.23×10^{-3}	9.51×10^{-3}	9.47×10^{-3}	8.98×10^{-3}	9.57×10^{-3}	9.54×10^{-3}
d_4	9.23×10^{-3}	9.51×10^{-3}	9.47×10^{-3}	8.98×10^{-3}	9.57×10^{-3}	9.54×10^{-3}
d_5	6.58×10^{-3}	6.58×10^{-3}	6.58×10^{-3}	6.58×10^{-3}	6.58×10^{-3}	6.58×10^{-3}
e_4	3.14×10^{-4}	3.17×10^{-4}	3.17×10^{-4}	3.09×10^{-4}	3.17×10^{-4}	3.17×10^{-4}
e_5	3.14×10^{-4}	3.17×10^{-4}	3.17×10^{-4}	3.09×10^{-4}	3.17×10^{-4}	3.17×10^{-4}
g_5	5.70×10^{-6}	5.71×10^{-6}	5.70×10^{-6}	5.72×10^{-6}	5.71×10^{-6}	5.71×10^{-6}
$RMSE_1$	42.471	42.782	42.652	42.471	43.051	42.911
$RMSE_2$	13.098	14.344	13.843	13.108	15.268	14.772
$RMSE_3$	5.301	6.001	5.739	5.337	6.353	6.117
$RMSE_4$	0.785	0.913	0.874	0.869	0.948	0.917
$RMSE_5$	0.107	0.125	0.120	0.147	0.128	0.125
Percent Error 1	12.453	11.607	11.809	12.472	11.296	12.472
Percent Error 2	4.085	2.664	2.992	4.208	3.494	4.208
Percent Error 3	1.424	1.191	1.113	1.624	1.271	1.624
Percent Error 4	0.196	0.183	0.173	0.323	0.190	0.323
Percent Error 5	0.043	0.041	0.038	0.101	0.043	0.101

Table B.39: Fitting coefficients and errors for the ACCQ basis set for the RHF γ_{zzzz} values at zero field.

ACCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	12.082	12.503	12.403	12.072	12.658	12.584
b_2	12.082	12.503	12.403	12.072	12.658	12.584
b_3	9.839	9.792	9.798	9.893	9.780	9.782
b_4	9.839	9.792	9.798	9.893	9.780	9.782
b_5	10.082	10.082	10.082	10.083	10.083	10.082
c_2	0.246	0.261	0.258	0.244	0.264	0.262
c_3	0.246	0.261	0.258	0.244	0.264	0.262
c_4	0.156	0.155	0.155	0.157	0.155	0.155
c_5	0.156	0.155	0.155	0.157	0.155	0.155
d_3	8.91×10^{-3}	9.19×10^{-3}	9.15×10^{-3}	8.65×10^{-3}	9.25×10^{-3}	9.22×10^{-3}
d_4	8.91×10^{-3}	9.19×10^{-3}	9.15×10^{-3}	8.65×10^{-3}	9.25×10^{-3}	9.22×10^{-3}
d_5	6.19×10^{-3}	6.19×10^{-3}	6.19×10^{-3}	6.18×10^{-3}	6.19×10^{-3}	6.19×10^{-3}
e_4	3.03×10^{-4}	3.06×10^{-4}	3.05×10^{-4}	2.97×10^{-4}	3.06×10^{-4}	3.06×10^{-4}
e_5	3.03×10^{-4}	3.06×10^{-4}	3.05×10^{-4}	2.97×10^{-4}	3.06×10^{-4}	3.06×10^{-4}
g_5	5.84×10^{-6}	5.84×10^{-6}	5.83×10^{-6}	5.87×10^{-6}	5.84×10^{-6}	5.83×10^{-6}
$RMSE_1$	47.962	48.221	48.113	47.963	48.445	48.329
$RMSE_2$	12.635	13.847	13.360	12.645	14.745	14.262
$RMSE_3$	5.117	5.797	5.543	5.154	6.139	5.909
$RMSE_4$	0.804	0.935	0.896	0.890	0.971	0.939
$RMSE_5$	1.18×10^{-1}	1.38×10^{-1}	1.33×10^{-1}	0.162	1.42×10^{-1}	1.38×10^{-1}
Percent Error 1	11.867	11.148	11.319	11.884	10.884	11.884
Percent Error 2	3.465	2.259	2.537	3.571	2.940	3.571
Percent Error 3	1.215	1.008	0.942	1.390	1.075	1.390
Percent Error 4	1.77×10^{-1}	1.65×10^{-1}	1.52×10^{-1}	2.93×10^{-1}	1.71×10^{-1}	2.93×10^{-1}
Percent Error 5	4.20×10^{-2}	4.05×10^{-2}	3.74×10^{-2}	0.101	4.20×10^{-2}	0.101

Table B.40: Fitting coefficients and errors for the DACCD basis set for the RHF γ_{zzzz} values at zero field.

DACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	15.058	15.520	15.410	15.049	15.691	15.609
b_2	15.058	15.520	15.410	15.049	15.691	15.609
b_3	12.554	12.512	12.517	12.602	12.501	12.504
b_4	12.554	12.512	12.517	12.602	12.501	12.504
b_5	12.767	12.766	12.767	12.765	12.766	12.766
c_2	0.309	0.322	0.319	0.307	0.326	0.323
c_3	0.309	0.322	0.319	0.307	0.326	0.323
c_4	0.226	0.225	0.225	0.228	0.225	0.225
c_5	0.226	0.225	0.225	0.228	0.225	0.225
d_3	9.95×10^{-3}	0.010	0.010	9.71×10^{-3}	0.010	0.010
d_4	9.95×10^{-3}	0.010	0.010	9.71×10^{-3}	0.010	0.010
d_5	7.57×10^{-3}	7.57×10^{-3}	7.57×10^{-3}	7.59×10^{-3}	7.58×10^{-3}	7.57×10^{-3}
e_4	2.78×10^{-4}	2.81×10^{-4}	2.81×10^{-4}	2.71×10^{-4}	2.81×10^{-4}	2.81×10^{-4}
e_5	2.78×10^{-4}	2.81×10^{-4}	2.81×10^{-4}	2.71×10^{-4}	2.81×10^{-4}	2.81×10^{-4}
g_5	5.11×10^{-6}	5.11×10^{-6}	5.12×10^{-6}	5.05×10^{-6}	5.10×10^{-6}	5.11×10^{-6}
$RMSE_1$	59.638	59.889	59.784	59.639	60.107	59.994
$RMSE_2$	13.725	14.982	14.475	13.733	15.940	15.434
$RMSE_3$	4.688	5.319	5.083	4.721	5.636	5.422
$RMSE_4$	0.710	0.827	0.792	0.791	0.859	0.831
$RMSE_5$	0.136	0.159	0.153	0.186	0.163	0.159
Percent Error 1	11.963	11.297	11.455	11.975	11.051	11.975
Percent Error 2	3.063	2.017	2.259	3.145	2.594	3.145
Percent Error 3	0.941	0.779	0.728	1.076	0.832	1.076
Percent Error 4	0.137	0.128	0.119	0.231	0.133	0.231
Percent Error 5	0.022	0.024	0.022	0.054	0.025	0.054

Table B.41: Fitting coefficients and errors for the DACCT basis set for the RHF γ_{zzzz} values at zero field.

DACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	13.468	13.938	13.826	13.459	14.111	14.028
b_2	13.468	13.938	13.826	13.459	14.111	14.028
b_3	10.928	10.885	10.890	10.977	10.874	10.876
b_4	10.928	10.885	10.890	10.977	10.874	10.876
b_5	11.148	11.148	11.148	11.146	11.147	11.148
c_2	0.285	0.300	0.297	0.282	0.304	0.301
c_3	0.285	0.300	0.297	0.282	0.304	0.301
c_4	0.189	0.188	0.188	0.190	0.188	0.188
c_5	0.189	0.188	0.188	0.190	0.188	0.188
d_3	0.010	0.010	0.010	9.85×10^{-3}	0.010	0.010
d_4	0.010	0.010	0.010	9.85×10^{-3}	0.010	0.010
d_5	7.63×10^{-3}	7.63×10^{-3}	7.63×10^{-3}	7.66×10^{-3}	7.64×10^{-3}	7.63×10^{-3}
e_4	3.21×10^{-4}	3.23×10^{-4}	3.23×10^{-4}	3.16×10^{-4}	3.24×10^{-4}	3.24×10^{-4}
e_5	3.21×10^{-4}	3.23×10^{-4}	3.23×10^{-4}	3.16×10^{-4}	3.24×10^{-4}	3.24×10^{-4}
g_5	5.28×10^{-6}	5.28×10^{-6}	5.29×10^{-6}	5.21×10^{-6}	5.27×10^{-6}	5.28×10^{-6}
$RMSE_1$	55.328	55.606	55.490	55.328	55.849	55.723
$RMSE_2$	14.159	15.472	14.943	14.168	16.458	15.933
$RMSE_3$	5.406	6.118	5.851	5.441	6.477	6.236
$RMSE_4$	0.728	0.848	0.812	0.808	0.881	0.853
$RMSE_5$	0.106	0.123	0.119	0.145	0.127	0.123
Percent Error 1	12.425	11.689	11.864	12.439	11.418	12.439
Percent Error 2	3.501	2.293	2.572	3.600	2.997	3.600
Percent Error 3	1.159	0.970	0.906	1.317	1.036	1.317
Percent Error 4	0.148	0.138	0.128	0.245	0.144	0.245
Percent Error 5	0.019	0.021	0.019	0.046	0.022	0.046

Table B.42: Fitting coefficients and errors for the PC3 basis set for the RHF γ_{zzzz} values at zero field.

PC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	4.545	5.011	4.900	4.536	5.184	5.101
b_2	4.545	5.011	4.900	4.536	5.184	5.101
b_3	2.027	1.983	1.988	2.077	1.971	1.974
b_4	2.027	1.983	1.988	2.077	1.971	1.974
b_5	2.252	2.252	2.252	2.250	2.251	2.252
c_2	0.164	0.179	0.176	0.161	0.183	0.181
c_3	0.164	0.179	0.176	0.161	0.183	0.181
c_4	0.065	0.065	0.065	0.066	0.065	0.065
c_5	0.065	0.065	0.065	0.066	0.065	0.065
d_3	0.010	0.010	0.010	9.75×10^{-3}	0.010	0.010
d_4	0.010	0.010	0.010	9.75×10^{-3}	0.010	0.010
d_5	7.49×10^{-3}	7.49×10^{-3}	7.49×10^{-3}	7.52×10^{-3}	7.49×10^{-3}	7.49×10^{-3}
e_4	3.29×10^{-4}	3.31×10^{-4}	3.31×10^{-4}	3.25×10^{-4}	3.32×10^{-4}	3.32×10^{-4}
e_5	3.29×10^{-4}	3.31×10^{-4}	3.31×10^{-4}	3.25×10^{-4}	3.32×10^{-4}	3.32×10^{-4}
g_5	5.40×10^{-6}	5.41×10^{-6}	5.41×10^{-6}	5.33×10^{-6}	5.40×10^{-6}	5.41×10^{-6}
$RMSE_1$	33.842	34.289	34.103	33.842	34.676	34.476
$RMSE_2$	14.108	15.424	14.894	14.118	16.408	15.883
$RMSE_3$	5.547	6.272	6.000	5.582	6.639	6.393
$RMSE_4$	0.742	0.865	0.828	0.822	0.899	0.869
$RMSE_5$	0.088	0.103	0.099	0.122	0.106	0.103
Percent Error 1	14.084	12.892	13.175	14.107	12.452	14.107
Percent Error 2	5.717	3.739	4.195	5.881	4.845	5.881
Percent Error 3	1.933	1.615	1.509	2.195	1.725	2.195
Percent Error 4	0.242	0.226	0.209	0.397	0.235	0.397
Percent Error 5	0.026	0.029	0.027	0.066	0.030	0.066

Table B.43: Fitting coefficients and errors for the APC3 basis set for the RHF γ_{zzzz} values at zero field.

APC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	13.702	14.164	14.054	13.693	14.335	14.253
b_2	13.702	14.164	14.054	13.693	14.335	14.253
b_3	11.210	11.166	11.171	11.262	11.154	11.156
b_4	11.210	11.166	11.171	11.262	11.154	11.156
b_5	11.439	11.439	11.439	11.438	11.439	11.439
c_2	0.275	0.290	0.286	0.272	0.293	0.291
c_3	0.275	0.290	0.286	0.272	0.293	0.291
c_4	0.183	0.183	0.183	0.185	0.183	0.183
c_5	0.183	0.183	0.183	0.185	0.183	0.183
d_3	9.90×10^{-3}	0.010	0.010	9.65×10^{-3}	0.010	0.010
d_4	9.90×10^{-3}	0.010	0.010	9.65×10^{-3}	0.010	0.010
d_5	7.34×10^{-3}	7.34×10^{-3}	7.33×10^{-3}	7.35×10^{-3}	7.34×10^{-3}	7.33×10^{-3}
e_4	3.06×10^{-4}	3.09×10^{-4}	3.08×10^{-4}	3.00×10^{-4}	3.09×10^{-4}	3.09×10^{-4}
e_5	3.06×10^{-4}	3.09×10^{-4}	3.08×10^{-4}	3.00×10^{-4}	3.09×10^{-4}	3.09×10^{-4}
g_5	5.51×10^{-6}	5.51×10^{-6}	5.51×10^{-6}	5.47×10^{-6}	5.50×10^{-6}	5.51×10^{-6}
$RMSE_1$	53.467	53.747	53.630	53.467	53.990	53.864
$RMSE_2$	13.833	15.122	14.603	13.843	16.092	15.576
$RMSE_3$	5.159	5.845	5.588	5.194	6.190	5.958
$RMSE_4$	0.761	0.885	0.848	0.844	0.920	0.890
$RMSE_5$	0.121	0.142	0.137	0.167	0.146	0.142
Percent Error 1	11.815	11.104	11.273	11.829	10.841	11.829
Percent Error 2	3.354	2.198	2.465	3.450	2.846	3.450
Percent Error 3	1.099	0.912	0.852	1.254	0.974	1.254
Percent Error 4	0.154	0.143	0.132	0.255	0.148	0.255
Percent Error 5	0.021	0.023	0.021	0.050	0.024	0.050

Table B.44: Fitting coefficients and errors for the APC4 basis set for the RHF γ_{zzzz} values at zero field.

APC4	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	13.762	14.214	14.107	13.753	14.381	14.301
b_2	13.762	14.214	14.107	13.753	14.381	14.301
b_3	11.330	11.286	11.290	11.381	11.274	11.276
b_4	11.330	11.286	11.290	11.381	11.274	11.276
b_5	11.559	11.558	11.559	11.558	11.558	11.559
c_2	0.279	0.294	0.291	0.277	0.298	0.295
c_3	0.279	0.294	0.291	0.277	0.298	0.295
c_4	0.187	0.186	0.186	0.188	0.186	0.186
c_5	0.187	0.186	0.186	0.188	0.186	0.186
d_3	9.66×10^{-3}	9.93×10^{-3}	9.89×10^{-3}	9.41×10^{-3}	9.98×10^{-3}	9.95×10^{-3}
d_4	9.66×10^{-3}	9.93×10^{-3}	9.89×10^{-3}	9.41×10^{-3}	9.98×10^{-3}	9.95×10^{-3}
d_5	7.10×10^{-3}	7.11×10^{-3}	7.10×10^{-3}	7.11×10^{-3}	7.11×10^{-3}	7.11×10^{-3}
e_4	3.10×10^{-4}	3.12×10^{-4}	3.12×10^{-4}	3.05×10^{-4}	3.12×10^{-4}	3.13×10^{-4}
e_5	3.10×10^{-4}	3.12×10^{-4}	3.12×10^{-4}	3.05×10^{-4}	3.12×10^{-4}	3.13×10^{-4}
g_5	5.50×10^{-6}	5.49×10^{-6}	5.50×10^{-6}	5.47×10^{-6}	5.48×10^{-6}	5.49×10^{-6}
$RMSE_1$	54.184	54.448	54.337	54.184	54.677	54.558
$RMSE_2$	13.574	14.847	14.334	13.584	15.800	15.291
$RMSE_3$	5.225	5.916	5.657	5.260	6.264	6.030
$RMSE_4$	0.757	0.882	0.845	0.840	0.917	0.887
$RMSE_5$	0.108	0.127	0.122	0.149	0.131	0.127
Percent Error 1	11.936	11.238	11.404	11.950	10.981	11.950
Percent Error 2	3.319	2.172	2.437	3.416	2.824	3.416
Percent Error 3	1.112	0.924	0.863	1.268	0.986	1.268
Percent Error 4	0.152	0.142	0.131	0.251	0.148	0.251
Percent Error 5	0.019	0.022	0.020	0.046	0.023	0.046

B.5 γ_{xxzz} Results

Table B.45: Fitting coefficients and errors for the CCD basis set for the RHF γ_{xxzz} values at zero field.

CCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	3.426	3.517	3.495	3.426	3.551	3.535
b_2	3.426	3.517	3.495	3.426	3.551	3.535
b_3	2.918	2.914	2.914	2.922	2.913	2.913
b_4	2.918	2.914	2.914	2.922	2.913	2.913
b_5	2.940	2.940	2.940	2.941	2.940	2.940
c_2	0.088	0.090	0.090	0.088	0.091	0.091
c_3	0.088	0.090	0.090	0.088	0.091	0.091
c_4	0.074	0.074	0.074	0.074	0.074	0.074
c_5	0.074	0.074	0.074	0.074	0.074	0.074
d_3	2.02×10^{-3}	2.04×10^{-3}	2.04×10^{-3}	2.00×10^{-3}	2.05×10^{-3}	2.05×10^{-3}
d_4	2.02×10^{-3}	2.04×10^{-3}	2.04×10^{-3}	2.00×10^{-3}	2.05×10^{-3}	2.05×10^{-3}
d_5	1.77×10^{-3}	1.77×10^{-3}	1.77×10^{-3}	1.76×10^{-3}	1.77×10^{-3}	1.77×10^{-3}
e_4	4.66×10^{-5}	4.65×10^{-5}	4.65×10^{-5}	4.68×10^{-5}	4.65×10^{-5}	4.65×10^{-5}
e_5	4.66×10^{-5}	4.65×10^{-5}	4.65×10^{-5}	4.68×10^{-5}	4.65×10^{-5}	4.65×10^{-5}
g_5	5.30×10^{-7}	5.30×10^{-7}	5.26×10^{-7}	5.69×10^{-7}	5.37×10^{-7}	5.29×10^{-7}
$RMSE_1$	16.791	16.825	16.811	16.791	16.856	16.840
$RMSE_2$	2.734	2.963	2.870	2.735	3.144	3.051
$RMSE_3$	0.781	0.877	0.841	0.784	0.927	0.894
$RMSE_4$	0.072	0.083	0.080	0.079	0.086	0.083
$RMSE_5$	4.74×10^{-3}	5.93×10^{-3}	5.56×10^{-3}	0.010	6.50×10^{-3}	5.86×10^{-3}
Percent Error 1	27.271	26.132	26.402	27.278	25.706	27.278
Percent Error 2	5.045	3.372	3.759	5.141	6.134	5.141
Percent Error 3	1.274	1.328	1.328	1.416	1.420	1.416
Percent Error 4	1.782	0.988	0.931	2.810	1.120	2.810
Percent Error 5	0.010	0.014	0.013	0.035	0.016	0.035

Table B.46: Fitting coefficients and errors for the CCT basis set for the RHF γ_{xxzz} values at zero field.

CCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	3.005	3.073	3.057	3.004	3.099	3.087
b_2	3.005	3.073	3.057	3.004	3.099	3.087
b_3	2.621	2.617	2.618	2.625	2.616	2.616
b_4	2.621	2.617	2.618	2.625	2.616	2.616
b_5	2.639	2.639	2.639	2.640	2.640	2.639
c_2	0.085	0.087	0.086	0.085	0.087	0.087
c_3	0.085	0.087	0.086	0.085	0.087	0.087
c_4	0.074	0.074	0.074	0.074	0.074	0.074
c_5	0.074	0.074	0.074	0.074	0.074	0.074
d_3	1.52×10^{-3}	1.55×10^{-3}	1.54×10^{-3}	1.51×10^{-3}	1.55×10^{-3}	1.55×10^{-3}
d_4	1.52×10^{-3}	1.55×10^{-3}	1.54×10^{-3}	1.51×10^{-3}	1.55×10^{-3}	1.55×10^{-3}
d_5	1.32×10^{-3}	1.32×10^{-3}	1.32×10^{-3}	1.31×10^{-3}	1.31×10^{-3}	1.32×10^{-3}
e_4	3.63×10^{-5}	3.62×10^{-5}	3.62×10^{-5}	3.67×10^{-5}	3.62×10^{-5}	3.61×10^{-5}
e_5	3.63×10^{-5}	3.62×10^{-5}	3.62×10^{-5}	3.67×10^{-5}	3.62×10^{-5}	3.61×10^{-5}
g_5	4.48×10^{-7}	4.48×10^{-7}	4.46×10^{-7}	4.68×10^{-7}	4.52×10^{-7}	4.47×10^{-7}
$RMSE_1$	16.091	16.111	16.103	16.091	16.129	16.120
$RMSE_2$	2.070	2.244	2.174	2.070	2.382	2.311
$RMSE_3$	0.609	0.683	0.655	0.612	0.721	0.696
$RMSE_4$	0.061	0.071	0.068	0.067	0.074	0.071
$RMSE_5$	6.82×10^{-3}	8.46×10^{-3}	8.04×10^{-3}	0.011	8.85×10^{-3}	8.42×10^{-3}
Percent Error 1	26.275	25.375	25.588	26.281	25.040	26.281
Percent Error 2	3.997	2.669	2.976	4.074	4.605	4.074
Percent Error 3	1.035	1.041	1.035	1.153	1.113	1.153
Percent Error 4	0.664	0.517	0.465	1.084	0.538	1.084
Percent Error 5	0.013	0.017	0.016	0.039	0.019	0.039

Table B.47: Fitting coefficients and errors for the CCQ basis set for the RHF γ_{xxzz} values at zero field.

CCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	2.975	3.041	3.025	2.975	3.065	3.053
b_2	2.975	3.041	3.025	2.975	3.065	3.053
b_3	2.612	2.608	2.608	2.616	2.607	2.607
b_4	2.612	2.608	2.608	2.616	2.607	2.607
b_5	2.631	2.632	2.631	2.633	2.632	2.632
c_2	0.088	0.089	0.089	0.088	0.090	0.090
c_3	0.088	0.089	0.089	0.088	0.090	0.090
c_4	0.080	0.080	0.080	0.081	0.080	0.080
c_5	0.080	0.080	0.080	0.081	0.080	0.080
d_3	1.44×10^{-3}	1.47×10^{-3}	1.46×10^{-3}	1.43×10^{-3}	1.47×10^{-3}	1.47×10^{-3}
d_4	1.44×10^{-3}	1.47×10^{-3}	1.46×10^{-3}	1.43×10^{-3}	1.47×10^{-3}	1.47×10^{-3}
d_5	1.22×10^{-3}	1.22×10^{-3}	1.22×10^{-3}	1.20×10^{-3}	1.22×10^{-3}	1.22×10^{-3}
e_4	2.58×10^{-5}	2.59×10^{-5}	2.59×10^{-5}	2.57×10^{-5}	2.60×10^{-5}	2.60×10^{-5}
e_5	2.58×10^{-5}	2.59×10^{-5}	2.59×10^{-5}	2.57×10^{-5}	2.60×10^{-5}	2.60×10^{-5}
g_5	4.75×10^{-7}	4.75×10^{-7}	4.70×10^{-7}	5.30×10^{-7}	4.84×10^{-7}	4.73×10^{-7}
$RMSE_1$	16.673	16.690	16.683	16.673	16.706	16.698
$RMSE_2$	1.924	2.085	2.019	1.924	2.214	2.148
$RMSE_3$	0.436	0.492	0.471	0.439	0.520	0.501
$RMSE_4$	0.065	0.074	0.071	0.070	0.077	0.075
$RMSE_5$	6.86×10^{-3}	7.85×10^{-3}	7.50×10^{-3}	1.29×10^{-2}	8.54×10^{-3}	7.79×10^{-3}
Percent Error 1	21.577	20.887	21.051	21.582	20.630	21.582
Percent Error 2	2.896	1.952	2.172	2.945	2.940	2.945
Percent Error 3	0.629	0.582	0.545	0.711	0.621	0.711
Percent Error 4	0.079	0.079	0.075	0.122	0.080	0.122
Percent Error 5	0.029	0.032	0.028	0.108	0.037	0.108

Table B.48: Fitting coefficients and errors for the ACCD basis set for the RHF γ_{xxzz} values at zero field.

ACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	6.471	6.524	6.512	6.470	6.544	6.535
b_2	6.471	6.524	6.512	6.470	6.544	6.535
b_3	6.178	6.174	6.175	6.183	6.173	6.173
b_4	6.178	6.174	6.175	6.183	6.173	6.173
b_5	6.199	6.199	6.199	6.199	6.199	6.199
c_2	0.121	0.122	0.122	0.120	0.123	0.123
c_3	0.121	0.122	0.122	0.120	0.123	0.123
c_4	0.109	0.109	0.109	0.109	0.109	0.109
c_5	0.109	0.109	0.109	0.109	0.109	0.109
d_3	1.16×10^{-3}	1.19×10^{-3}	1.18×10^{-3}	1.14×10^{-3}	1.19×10^{-3}	1.19×10^{-3}
d_4	1.16×10^{-3}	1.19×10^{-3}	1.18×10^{-3}	1.14×10^{-3}	1.19×10^{-3}	1.19×10^{-3}
d_5	9.31×10^{-4}	9.31×10^{-4}	9.31×10^{-4}	9.30×10^{-4}	9.31×10^{-4}	9.31×10^{-4}
e_4	3.85×10^{-5}	3.85×10^{-5}	3.85×10^{-5}	3.84×10^{-5}	3.86×10^{-5}	3.86×10^{-5}
e_5	3.85×10^{-5}	3.85×10^{-5}	3.85×10^{-5}	3.84×10^{-5}	3.86×10^{-5}	3.86×10^{-5}
g_5	4.97×10^{-7}	4.98×10^{-7}	4.97×10^{-7}	5.02×10^{-7}	4.99×10^{-7}	4.98×10^{-7}
$RMSE_1$	22.720	22.729	22.725	22.720	22.737	22.733
$RMSE_2$	1.641	1.789	1.729	1.642	1.901	1.842
$RMSE_3$	0.646	0.728	0.697	0.649	0.769	0.742
$RMSE_4$	0.068	0.079	0.076	0.075	0.082	0.079
$RMSE_5$	3.07×10^{-3}	3.39×10^{-3}	3.30×10^{-3}	3.84×10^{-3}	3.47×10^{-3}	3.40×10^{-3}
Percent Error 1	13.482	13.213	13.276	13.486	13.113	13.486
Percent Error 2	1.300	0.852	0.955	1.335	1.173	1.335
Percent Error 3	0.431	0.374	0.349	0.483	0.400	0.483
Percent Error 4	0.040	0.039	0.036	0.064	0.039	0.064
Percent Error 5	4.85×10^{-3}	4.58×10^{-3}	4.16×10^{-3}	0.012	4.82×10^{-3}	0.012

Table B.49: Fitting coefficients and errors for the ACCT basis set for the RHF γ_{xxzz} values at zero field.

ACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	6.749	6.815	6.800	6.749	6.840	6.828
b_2	6.749	6.815	6.800	6.749	6.840	6.828
b_3	6.388	6.383	6.383	6.393	6.382	6.382
b_4	6.388	6.383	6.383	6.393	6.382	6.382
b_5	6.413	6.413	6.413	6.413	6.413	6.413
c_2	0.131	0.132	0.132	0.131	0.133	0.133
c_3	0.131	0.132	0.132	0.131	0.133	0.133
c_4	0.120	0.120	0.120	0.120	0.120	0.120
c_5	0.120	0.120	0.120	0.120	0.120	0.120
d_3	1.44×10^{-3}	1.47×10^{-3}	1.46×10^{-3}	1.41×10^{-3}	1.47×10^{-3}	1.47×10^{-3}
d_4	1.44×10^{-3}	1.47×10^{-3}	1.46×10^{-3}	1.41×10^{-3}	1.47×10^{-3}	1.47×10^{-3}
d_5	1.16×10^{-3}	1.16×10^{-3}	1.16×10^{-3}	1.16×10^{-3}	1.16×10^{-3}	1.16×10^{-3}
e_4	3.48×10^{-5}	3.48×10^{-5}	3.48×10^{-5}	3.46×10^{-5}	3.49×10^{-5}	3.49×10^{-5}
e_5	3.48×10^{-5}	3.48×10^{-5}	3.48×10^{-5}	3.46×10^{-5}	3.49×10^{-5}	3.49×10^{-5}
g_5	6.03×10^{-7}	6.04×10^{-7}	6.03×10^{-7}	6.07×10^{-7}	6.05×10^{-7}	6.04×10^{-7}
$RMSE_1$	24.638	24.650	24.645	24.638	24.661	24.656
$RMSE_2$	1.953	2.125	2.055	1.954	2.258	2.189
$RMSE_3$	0.586	0.661	0.633	0.589	0.699	0.673
$RMSE_4$	0.082	0.095	0.092	0.091	0.099	0.096
$RMSE_5$	3.82×10^{-3}	4.50×10^{-3}	4.32×10^{-3}	5.31×10^{-3}	4.65×10^{-3}	4.50×10^{-3}
Percent Error 1	12.844	12.553	12.622	12.848	12.445	12.848
Percent Error 2	1.292	0.859	0.959	1.321	1.167	1.321
Percent Error 3	0.352	0.299	0.279	0.399	0.319	0.399
Percent Error 4	0.043	0.041	0.038	0.068	0.041	0.068
Percent Error 5	5.60×10^{-3}	5.82×10^{-3}	5.22×10^{-3}	0.014	6.23×10^{-3}	0.014

Table B.50: Fitting coefficients and errors for the ACCQ basis set for the RHF γ_{xxzz} values at zero field.

ACCQ	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	7.530	7.600	7.583	7.529	7.625	7.613
b_2	7.530	7.600	7.583	7.529	7.625	7.613
b_3	7.149	7.144	7.144	7.154	7.142	7.143
b_4	7.149	7.144	7.144	7.154	7.142	7.143
b_5	7.175	7.175	7.175	7.175	7.175	7.175
c_2	0.138	0.140	0.140	0.138	0.140	0.140
c_3	0.138	0.140	0.140	0.138	0.140	0.140
c_4	0.129	0.129	0.129	0.129	0.129	0.129
c_5	0.129	0.129	0.129	0.129	0.129	0.129
d_3	1.52×10^{-3}	1.55×10^{-3}	1.54×10^{-3}	1.49×10^{-3}	1.55×10^{-3}	1.55×10^{-3}
d_4	1.52×10^{-3}	1.55×10^{-3}	1.54×10^{-3}	1.49×10^{-3}	1.55×10^{-3}	1.55×10^{-3}
d_5	1.23×10^{-3}	1.23×10^{-3}	1.23×10^{-3}	1.21×10^{-3}	1.22×10^{-3}	1.23×10^{-3}
e_4	3.28×10^{-5}	3.32×10^{-5}	3.32×10^{-5}	3.20×10^{-5}	3.33×10^{-5}	3.33×10^{-5}
e_5	3.28×10^{-5}	3.32×10^{-5}	3.32×10^{-5}	3.20×10^{-5}	3.33×10^{-5}	3.33×10^{-5}
g_5	6.21×10^{-7}	6.21×10^{-7}	6.18×10^{-7}	6.52×10^{-7}	6.25×10^{-7}	6.20×10^{-7}
$RMSE_1$	26.080	26.093	26.087	26.080	26.104	26.098
$RMSE_2$	2.043	2.221	2.148	2.043	2.360	2.288
$RMSE_3$	0.555	0.630	0.602	0.559	0.667	0.642
$RMSE_4$	0.087	0.100	0.096	0.096	0.104	0.100
$RMSE_5$	0.018	0.021	0.020	0.025	0.022	0.021
Percent Error 1	11.828	11.562	11.625	11.832	11.462	11.832
Percent Error 2	1.163	0.776	0.866	1.189	1.029	1.189
Percent Error 3	0.298	0.250	0.233	0.340	0.266	0.340
Percent Error 4	0.044	0.041	0.039	0.073	0.042	0.073
Percent Error 5	0.021	0.020	0.018	0.054	0.021	0.054

Table B.51: Fitting coefficients and errors for the DACCD basis set for the RHF γ_{xxzz} values at zero field.

DACCD	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	8.664	8.729	8.713	8.663	8.752	8.741
b_2	8.664	8.729	8.713	8.663	8.752	8.741
b_3	8.318	8.312	8.313	8.326	8.311	8.311
b_4	8.318	8.312	8.313	8.326	8.311	8.311
b_5	8.351	8.351	8.351	8.351	8.351	8.351
c_2	0.154	0.156	0.156	0.154	0.157	0.156
c_3	0.154	0.156	0.156	0.154	0.157	0.156
c_4	0.143	0.143	0.143	0.143	0.143	0.143
c_5	0.143	0.143	0.143	0.143	0.143	0.143
d_3	1.37×10^{-3}	1.41×10^{-3}	1.41×10^{-3}	1.34×10^{-3}	1.42×10^{-3}	1.41×10^{-3}
d_4	1.37×10^{-3}	1.41×10^{-3}	1.41×10^{-3}	1.34×10^{-3}	1.42×10^{-3}	1.41×10^{-3}
d_5	1.02×10^{-3}	1.01×10^{-3}	1.02×10^{-3}	1.01×10^{-3}	1.01×10^{-3}	1.01×10^{-3}
e_4	3.75×10^{-5}	3.76×10^{-5}	3.76×10^{-5}	3.74×10^{-5}	3.76×10^{-5}	3.76×10^{-5}
e_5	3.75×10^{-5}	3.76×10^{-5}	3.76×10^{-5}	3.74×10^{-5}	3.76×10^{-5}	3.76×10^{-5}
g_5	7.71×10^{-7}	7.71×10^{-7}	7.71×10^{-7}	7.75×10^{-7}	7.72×10^{-7}	7.71×10^{-7}
$RMSE_1$	29.054	29.064	29.059	29.054	29.072	29.068
$RMSE_2$	1.892	2.064	1.994	1.893	2.197	2.127
$RMSE_3$	0.635	0.716	0.686	0.640	0.757	0.730
$RMSE_4$	0.105	0.122	0.117	0.116	0.127	0.123
$RMSE_5$	2.95×10^{-3}	3.57×10^{-3}	3.41×10^{-3}	4.32×10^{-3}	3.70×10^{-3}	3.56×10^{-3}
Percent Error 1	11.281	11.066	11.117	11.285	10.987	11.285
Percent Error 2	0.973	0.643	0.719	0.997	0.835	0.997
Percent Error 3	0.293	0.244	0.228	0.335	0.260	0.335
Percent Error 4	0.041	0.038	0.036	0.065	0.039	0.065
Percent Error 5	3.30×10^{-3}	3.55×10^{-3}	3.20×10^{-3}	8.52×10^{-3}	3.80×10^{-3}	8.52×10^{-3}

Table B.52: Fitting coefficients and errors for the DACCT basis set for the RHF γ_{xxzz} values at zero field.

DACCT	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	8.791	8.861	8.845	8.790	8.887	8.875
b_2	8.791	8.861	8.845	8.790	8.887	8.875
b_3	8.408	8.403	8.404	8.414	8.402	8.402
b_4	8.408	8.403	8.404	8.414	8.402	8.402
b_5	8.435	8.435	8.435	8.435	8.435	8.435
c_2	0.151	0.153	0.152	0.151	0.153	0.153
c_3	0.151	0.153	0.152	0.151	0.153	0.153
c_4	0.140	0.139	0.139	0.140	0.139	0.139
c_5	0.140	0.139	0.139	0.140	0.139	0.139
d_3	1.52×10^{-3}	1.55×10^{-3}	1.55×10^{-3}	1.49×10^{-3}	1.56×10^{-3}	1.56×10^{-3}
d_4	1.52×10^{-3}	1.55×10^{-3}	1.55×10^{-3}	1.49×10^{-3}	1.56×10^{-3}	1.56×10^{-3}
d_5	1.22×10^{-3}	1.22×10^{-3}	1.22×10^{-3}	1.22×10^{-3}	1.22×10^{-3}	1.22×10^{-3}
e_4	3.82×10^{-5}	3.85×10^{-5}	3.85×10^{-5}	3.76×10^{-5}	3.86×10^{-5}	3.86×10^{-5}
e_5	3.82×10^{-5}	3.85×10^{-5}	3.85×10^{-5}	3.76×10^{-5}	3.86×10^{-5}	3.86×10^{-5}
g_5	6.49×10^{-7}	6.49×10^{-7}	6.49×10^{-7}	6.51×10^{-7}	6.50×10^{-7}	6.49×10^{-7}
$RMSE_1$	28.424	28.436	28.431	28.424	28.447	28.441
$RMSE_2$	2.076	2.260	2.186	2.077	2.402	2.328
$RMSE_3$	0.644	0.729	0.698	0.649	0.772	0.744
$RMSE_4$	0.090	0.104	0.100	0.099	0.108	0.105
$RMSE_5$	0.014	0.016	0.015	0.019	0.016	0.016
Percent Error 1	11.153	10.920	10.975	11.157	10.833	11.157
Percent Error 2	1.050	0.696	0.778	1.076	0.926	1.076
Percent Error 3	0.296	0.247	0.231	0.337	0.264	0.337
Percent Error 4	0.039	0.036	0.034	0.064	0.037	0.064
Percent Error 5	0.013	0.012	0.011	0.030	0.013	0.030

Table B.53: Fitting coefficients and errors for the PC3 basis set for the RHF γ_{xxzz} values at zero field.

PC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	5.666	5.727	5.713	5.665	5.750	5.739
b_2	5.666	5.727	5.713	5.665	5.750	5.739
b_3	5.326	5.322	5.323	5.331	5.321	5.321
b_4	5.326	5.322	5.323	5.331	5.321	5.321
b_5	5.349	5.349	5.349	5.351	5.350	5.349
c_2	0.110	0.111	0.111	0.109	0.111	0.111
c_3	0.110	0.111	0.111	0.109	0.111	0.111
c_4	0.102	0.102	0.102	0.102	0.102	0.102
c_5	0.102	0.102	0.102	0.102	0.102	0.102
d_3	1.35×10^{-3}	1.37×10^{-3}	1.37×10^{-3}	1.33×10^{-3}	1.38×10^{-3}	1.37×10^{-3}
d_4	1.35×10^{-3}	1.37×10^{-3}	1.37×10^{-3}	1.33×10^{-3}	1.38×10^{-3}	1.37×10^{-3}
d_5	1.10×10^{-3}	1.10×10^{-3}	1.10×10^{-3}	1.06×10^{-3}	1.09×10^{-3}	1.10×10^{-3}
e_4	2.52×10^{-5}	2.58×10^{-5}	2.58×10^{-5}	2.38×10^{-5}	2.59×10^{-5}	2.60×10^{-5}
e_5	2.52×10^{-5}	2.58×10^{-5}	2.58×10^{-5}	2.38×10^{-5}	2.59×10^{-5}	2.60×10^{-5}
g_5	5.40×10^{-7}	5.38×10^{-7}	5.31×10^{-7}	6.35×10^{-7}	5.50×10^{-7}	5.34×10^{-7}
$RMSE_1$	20.652	20.665	20.660	20.652	20.676	20.670
$RMSE_2$	1.801	1.956	1.893	1.801	2.078	2.015
$RMSE_3$	0.428	0.490	0.466	0.431	0.520	0.499
$RMSE_4$	0.080	0.091	0.088	0.090	0.094	0.092
$RMSE_5$	0.032	0.037	0.036	0.045	0.038	0.037
Percent Error 1	12.747	12.428	12.504	12.750	12.309	12.750
Percent Error 2	1.359	0.910	1.014	1.388	1.212	1.388
Percent Error 3	0.320	0.272	0.254	0.367	0.289	0.367
Percent Error 4	0.057	0.053	0.051	0.099	0.055	0.099
Percent Error 5	0.051	0.050	0.045	0.146	0.053	0.146

Table B.54: Fitting coefficients and errors for the APC3 basis set for the RHF γ_{xxzz} values at zero field.

APC3	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	8.829	8.896	8.880	8.828	8.921	8.909
b_2	8.829	8.896	8.880	8.828	8.921	8.909
b_3	8.463	8.458	8.458	8.469	8.457	8.457
b_4	8.463	8.458	8.458	8.469	8.457	8.457
b_5	8.489	8.489	8.489	8.489	8.489	8.489
c_2	0.150	0.152	0.151	0.150	0.152	0.152
c_3	0.150	0.152	0.151	0.150	0.152	0.152
c_4	0.139	0.139	0.139	0.139	0.139	0.139
c_5	0.139	0.139	0.139	0.139	0.139	0.139
d_3	1.45×10^{-3}	1.48×10^{-3}	1.48×10^{-3}	1.43×10^{-3}	1.49×10^{-3}	1.49×10^{-3}
d_4	1.45×10^{-3}	1.48×10^{-3}	1.48×10^{-3}	1.43×10^{-3}	1.49×10^{-3}	1.49×10^{-3}
d_5	1.16×10^{-3}	1.16×10^{-3}	1.16×10^{-3}	1.17×10^{-3}	1.16×10^{-3}	1.16×10^{-3}
e_4	3.69×10^{-5}	3.73×10^{-5}	3.72×10^{-5}	3.61×10^{-5}	3.73×10^{-5}	3.73×10^{-5}
e_5	3.69×10^{-5}	3.73×10^{-5}	3.72×10^{-5}	3.61×10^{-5}	3.73×10^{-5}	3.73×10^{-5}
g_5	6.26×10^{-7}	6.26×10^{-7}	6.26×10^{-7}	6.18×10^{-7}	6.24×10^{-7}	6.26×10^{-7}
$RMSE_1$	28.225	28.236	28.231	28.225	28.246	28.241
$RMSE_2$	1.986	2.162	2.091	1.986	2.299	2.227
$RMSE_3$	0.622	0.705	0.674	0.626	0.746	0.718
$RMSE_4$	0.087	0.101	0.097	0.097	0.105	0.102
$RMSE_5$	0.017	0.019	0.018	0.022	0.019	0.019
Percent Error 1	10.982	10.760	10.813	10.986	10.678	10.986
Percent Error 2	1.002	0.664	0.742	1.027	0.858	1.027
Percent Error 3	0.285	0.238	0.222	0.325	0.254	0.325
Percent Error 4	0.038	0.036	0.033	0.064	0.037	0.064
Percent Error 5	5.89×10^{-3}	6.34×10^{-3}	5.85×10^{-3}	0.014	6.57×10^{-3}	0.014

Table B.55: Fitting coefficients and errors for the APC4 basis set for the RHF γ_{xxzz} values at zero field.

APC4	All Points	0,5,10,15,20	0,4,8,12,16,20	0,6,12,18	0,7,14,20	0,3,9,15,20
b_1	8.828	8.894	8.879	8.827	8.919	8.907
b_2	8.828	8.894	8.879	8.827	8.919	8.907
b_3	8.466	8.460	8.461	8.473	8.458	8.459
b_4	8.466	8.460	8.461	8.473	8.458	8.459
b_5	8.496	8.497	8.496	8.496	8.496	8.496
c_2	0.151	0.152	0.152	0.150	0.153	0.153
c_3	0.151	0.152	0.152	0.150	0.153	0.153
c_4	0.140	0.140	0.140	0.140	0.140	0.140
c_5	0.140	0.140	0.140	0.140	0.140	0.140
d_3	1.44×10^{-3}	1.47×10^{-3}	1.47×10^{-3}	1.40×10^{-3}	1.48×10^{-3}	1.47×10^{-3}
d_4	1.44×10^{-3}	1.47×10^{-3}	1.47×10^{-3}	1.40×10^{-3}	1.48×10^{-3}	1.47×10^{-3}
d_5	1.10×10^{-3}	1.10×10^{-3}	1.10×10^{-3}	1.11×10^{-3}	1.10×10^{-3}	1.10×10^{-3}
e_4	3.58×10^{-5}	3.63×10^{-5}	3.62×10^{-5}	3.49×10^{-5}	3.64×10^{-5}	3.64×10^{-5}
e_5	3.58×10^{-5}	3.63×10^{-5}	3.62×10^{-5}	3.49×10^{-5}	3.64×10^{-5}	3.64×10^{-5}
g_5	7.19×10^{-7}	7.27×10^{-7}	7.21×10^{-7}	6.99×10^{-7}	7.30×10^{-7}	7.28×10^{-7}
$RMSE_1$	28.360	28.371	28.366	28.360	28.381	28.376
$RMSE_2$	1.959	2.135	2.064	1.960	2.270	2.199
$RMSE_3$	0.606	0.687	0.657	0.610	0.727	0.700
$RMSE_4$	0.100	0.115	0.111	0.110	0.120	0.116
$RMSE_5$	0.019	0.021	0.021	0.025	0.022	0.022
Percent Error 1	11.010	10.789	10.841	11.013	10.707	11.013
Percent Error 2	0.990	0.656	0.734	1.014	0.843	1.014
Percent Error 3	0.283	0.236	0.222	0.323	0.252	0.323
Percent Error 4	0.043	0.041	0.040	0.072	0.041	0.072
Percent Error 5	0.016	0.016	0.014	0.015	0.016	0.015

C Dimer Fitting Results

C.1 Energies of the T-Shaped Dimer

Table C.1: The energies of the T-shaped dimer at the different C-C distances for the CCSD level of theory using the ACCT basis set.

Field Strength	$r = 3.0$ Å	$r = 3.5$ Å	$r = 4.0$ Å	$r = 4.5$ Å	$r = 5.0$ Å
−0.005	−376.560 694	−376.615 955	−376.623 407	−376.623 362	−376.622 769
−0.004	−376.560 873	−376.615 938	−376.623 313	−376.623 232	−376.622 621
−0.003	−376.561 098	−376.615 964	−376.623 261	−376.623 144	−376.622 515
−0.002	−376.561 369	−376.616 032	−376.623 251	−376.623 097	−376.622 449
−0.001	−376.561 685	−376.616 144	−376.623 283	−376.623 091	−376.622 423
0	−376.562 047	−376.616 300	−376.623 358	−376.623 126	−376.622 438
0.001	−376.562 455	−376.616 498	−376.623 474	−376.623 203	−376.622 494
0.002	−376.562 908	−376.616 739	−376.623 632	−376.623 320	−376.622 590
0.003	−376.563 407	−376.617 024	−376.623 833	−376.623 480	−376.622 727
0.004	−376.563 952	−376.617 352	−376.624 075	−376.623 680	−376.622 904
0.005	−376.564 542	−376.617 723	−376.624 360	−376.623 921	−376.623 123
	$r = 5.5$ Å	$r = 6.0$ Å	$r = 6.5$ Å	$r = 7.0$ Å	$r = 7.5$ Å
−0.005	−376.622 392	−376.622 192	−376.622 080	−376.622 011	−376.621 969
−0.004	−376.622 235	−376.622 029	−376.621 914	−376.621 843	−376.621 799
−0.003	−376.622 118	−376.621 906	−376.621 787	−376.621 713	−376.621 667
−0.002	−376.622 041	−376.621 823	−376.621 700	−376.621 623	−376.621 576
−0.001	−376.622 005	−376.621 780	−376.621 652	−376.621 573	−376.621 523
0	−376.622 008	−376.621 776	−376.621 644	−376.621 562	−376.621 510
0.001	−376.622 052	−376.621 812	−376.621 676	−376.621 590	−376.621 536
0.002	−376.622 136	−376.621 888	−376.621 747	−376.621 658	−376.621 602
0.003	−376.622 260	−376.622 004	−376.621 858	−376.621 765	−376.621 707
0.004	−376.622 424	−376.622 160	−376.622 008	−376.621 912	−376.621 851
0.005	−376.622 628	−376.622 356	−376.622 198	−376.622 098	−376.622 035
	$r = 8.0$ Å	$r = 8.5$ Å	$r = 9.0$ Å	$r = 9.5$ Å	$r = 10.0$ Å
−0.005	−376.621 943	−376.621 924	−376.621 911	−376.621 902	−376.621 895
−0.004	−376.621 771	−376.621 752	−376.621 738	−376.621 728	−376.621 722
−0.003	−376.621 639	−376.621 619	−376.621 604	−376.621 594	−376.621 587
−0.002	−376.621 546	−376.621 525	−376.621 509	−376.621 498	−376.621 491
−0.001	−376.621 492	−376.621 470	−376.621 454	−376.621 442	−376.621 435
0	−376.621 477	−376.621 454	−376.621 437	−376.621 425	−376.621 417
0.001	−376.621 502	−376.621 478	−376.621 460	−376.621 447	−376.621 439
0.002	−376.621 566	−376.621 540	−376.621 522	−376.621 509	−376.621 499
0.003	−376.621 669	−376.621 642	−376.621 623	−376.621 609	−376.621 599
0.004	−376.621 811	−376.621 783	−376.621 763	−376.621 748	−376.621 738
0.005	−376.621 993	−376.621 964	−376.621 942	−376.621 927	−376.621 916

Table C.1: The energies of the T-shaped dimer at the different C-C distances for the CCSD level of theory using the ACCT basis set (continued).

Field Strength	$r = 10.5$ Å	$r = 11.0$ Å	$r = 11.5$ Å	$r = 12.0$ Å	$r = 12.5$ Å
−0.005	−376.621 892	−376.621 889	−376.621 888	−376.621 887	−376.621 886
−0.004	−376.621 718	−376.621 715	−376.621 714	−376.621 712	−376.621 712
−0.003	−376.621 583	−376.621 580	−376.621 578	−376.621 577	−376.621 576
−0.002	−376.621 487	−376.621 484	−376.621 482	−376.621 480	−376.621 479
−0.001	−376.621 430	−376.621 427	−376.621 425	−376.621 423	−376.621 422
0	−376.621 412	−376.621 409	−376.621 406	−376.621 404	−376.621 403
0.001	−376.621 433	−376.621 429	−376.621 427	−376.621 425	−376.621 423
0.002	−376.621 493	−376.621 489	−376.621 486	−376.621 484	−376.621 483
0.003	−376.621 593	−376.621 588	−376.621 585	−376.621 583	−376.621 581
0.004	−376.621 731	−376.621 726	−376.621 723	−376.621 720	−376.621 718
0.005	−376.621 908	−376.621 903	−376.621 899	−376.621 897	−376.621 894
	$r = 13.0$ Å	$r = 13.5$ Å	$r = 14.0$ Å	$r = 14.5$ Å	$r = 15.0$ Å
−0.005	−376.621 886	−376.621 885	−376.621 885	−376.621 885	−376.621 884
−0.004	−376.621 711	−376.621 711	−376.621 710	−376.621 710	−376.621 710
−0.003	−376.621 575	−376.621 575	−376.621 574	−376.621 574	−376.621 574
−0.002	−376.621 479	−376.621 478	−376.621 478	−376.621 477	−376.621 477
−0.001	−376.621 421	−376.621 420	−376.621 420	−376.621 419	−376.621 419
0	−376.621 402	−376.621 401	−376.621 401	−376.621 400	−376.621 400
0.001	−376.621 422	−376.621 421	−376.621 421	−376.621 420	−376.621 420
0.002	−376.621 481	−376.621 480	−376.621 480	−376.621 479	−376.621 479
0.003	−376.621 580	−376.621 578	−376.621 578	−376.621 577	−376.621 576
0.004	−376.621 717	−376.621 715	−376.621 714	−376.621 714	−376.621 713
0.005	−376.621 893	−376.621 891	−376.621 890	−376.621 889	−376.621 888

Table C.2: The energies of the T-shaped dimer at the different C-C distances for the CCSD(T) level of theory using the ACCT basis set.

Field Strength	$r = 3.0$ Å	$r = 3.5$ Å	$r = 4.0$ Å	$r = 4.5$ Å	$r = 5.0$ Å
−0.005	−376.621 711	−376.676 147	−376.683 178	−376.682 936	−376.682 256
−0.004	−376.621 881	−376.676 124	−376.683 080	−376.682 803	−376.682 105
−0.003	−376.622 096	−376.676 146	−376.683 024	−376.682 711	−376.681 996
−0.002	−376.622 359	−376.676 211	−376.683 011	−376.682 662	−376.681 928
−0.001	−376.622 667	−376.676 320	−376.683 041	−376.682 654	−376.681 901
0	−376.623 023	−376.676 473	−376.683 114	−376.682 688	−376.681 915
0.001	−376.623 425	−376.676 670	−376.683 229	−376.682 764	−376.681 970
0.002	−376.623 873	−376.676 910	−376.683 387	−376.682 882	−376.682 067
0.003	−376.624 368	−376.677 195	−376.683 588	−376.683 041	−376.682 204
0.004	−376.624 910	−376.677 523	−376.683 832	−376.683 243	−376.682 383
0.005	−376.625 498	−376.677 896	−376.684 118	−376.683 486	−376.682 603
	$r = 5.5$ Å	$r = 6.0$ Å	$r = 6.5$ Å	$r = 7.0$ Å	$r = 7.5$ Å
−0.005	−376.681 840	−376.681 623	−376.681 502	−376.681 429	−376.681 384
−0.004	−376.681 680	−376.681 457	−376.681 333	−376.681 257	−376.681 211
−0.003	−376.681 561	−376.681 332	−376.681 204	−376.681 126	−376.681 078
−0.002	−376.681 482	−376.681 247	−376.681 115	−376.681 034	−376.680 984
−0.001	−376.681 444	−376.681 202	−376.681 067	−376.680 983	−376.680 931
0	−376.681 447	−376.681 198	−376.681 058	−376.680 971	−376.680 918
0.001	−376.681 491	−376.681 234	−376.681 090	−376.681 000	−376.680 944
0.002	−376.681 575	−376.681 311	−376.681 161	−376.681 068	−376.681 010
0.003	−376.681 700	−376.681 428	−376.681 273	−376.681 177	−376.681 116
0.004	−376.681 865	−376.681 585	−376.681 425	−376.681 325	−376.681 262
0.005	−376.682 071	−376.681 783	−376.681 617	−376.681 514	−376.681 448
	$r = 8.0$ Å	$r = 8.5$ Å	$r = 9.0$ Å	$r = 9.5$ Å	$r = 10.0$ Å
−0.005	−376.681 356	−376.681 337	−376.681 323	−376.681 313	−376.681 307
−0.004	−376.681 182	−376.681 162	−376.681 147	−376.681 137	−376.681 130
−0.003	−376.681 048	−376.681 027	−376.681 012	−376.681 001	−376.680 994
−0.002	−376.680 953	−376.680 931	−376.680 916	−376.680 904	−376.680 897
−0.001	−376.680 898	−376.680 876	−376.680 859	−376.680 847	−376.680 840
0	−376.680 884	−376.680 860	−376.680 842	−376.680 830	−376.680 822
0.001	−376.680 908	−376.680 883	−376.680 865	−376.680 852	−376.680 844
0.002	−376.680 973	−376.680 947	−376.680 928	−376.680 914	−376.680 905
0.003	−376.681 077	−376.681 050	−376.681 030	−376.681 016	−376.681 006
0.004	−376.681 221	−376.681 193	−376.681 172	−376.681 157	−376.681 146
0.005	−376.681 405	−376.681 375	−376.681 353	−376.681 337	−376.681 326

Table C.2: The energies of the T-shaped dimer at the different C-C distances for the CCSD(T) level of theory using the ACCT basis set (continued).

Field Strength	$r = 10.5$ Å	$r = 11.0$ Å	$r = 11.5$ Å	$r = 12.0$ Å	$r = 12.5$ Å
−0.005	−376.681 303	−376.681 300	−376.681 299	−376.681 298	−376.681 297
−0.004	−376.681 126	−376.681 124	−376.681 122	−376.681 121	−376.681 120
−0.003	−376.680 990	−376.680 987	−376.680 985	−376.680 984	−376.680 983
−0.002	−376.680 892	−376.680 889	−376.680 887	−376.680 886	−376.680 885
−0.001	−376.680 835	−376.680 831	−376.680 829	−376.680 828	−376.680 826
0	−376.680 817	−376.680 813	−376.680 811	−376.680 809	−376.680 808
0.001	−376.680 838	−376.680 834	−376.680 831	−376.680 830	−376.680 828
0.002	−376.680 899	−376.680 895	−376.680 892	−376.680 890	−376.680 888
0.003	−376.680 999	−376.680 995	−376.680 992	−376.680 989	−376.680 988
0.004	−376.681 139	−376.681 135	−376.681 131	−376.681 129	−376.681 127
0.005	−376.681 319	−376.681 314	−376.681 310	−376.681 307	−376.681 305
	$r = 13.0$ Å	$r = 13.5$ Å	$r = 14.0$ Å	$r = 14.5$ Å	$r = 15.0$ Å
−0.005	−376.681 296	−376.681 296	−376.681 296	−376.681 295	−376.681 295
−0.004	−376.681 119	−376.681 119	−376.681 119	−376.681 118	−376.681 118
−0.003	−376.680 982	−376.680 982	−376.680 981	−376.680 981	−376.680 981
−0.002	−376.680 884	−376.680 884	−376.680 883	−376.680 883	−376.680 882
−0.001	−376.680 826	−376.680 825	−376.680 824	−376.680 824	−376.680 824
0	−376.680 807	−376.680 806	−376.680 805	−376.680 805	−376.680 804
0.001	−376.680 827	−376.680 826	−376.680 825	−376.680 825	−376.680 824
0.002	−376.680 887	−376.680 886	−376.680 885	−376.680 884	−376.680 884
0.003	−376.680 986	−376.680 985	−376.680 984	−376.680 983	−376.680 983
0.004	−376.681 125	−376.681 124	−376.681 123	−376.681 122	−376.681 121
0.005	−376.681 303	−376.681 302	−376.681 301	−376.681 300	−376.681 299

C.2 Fitting Coefficients

Table C.3: The fitting results for the RHF *ab initio* dipole moments of the CO_2 dimer using the ACCT basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	49.010	−1.074	0.085	−0.389	8.57×10^{-5}	1.99×10^{-4}	0.0158
5.0	37.555	−1.030	0.061	−0.374	1.24×10^{-4}	5.09×10^{-4}	0.0114
5.5	29.276	−0.991	0.045	−0.360	2.28×10^{-4}	1.04×10^{-3}	8.21×10^{-3}
6.0	23.227	−0.956	0.034	−0.348	3.72×10^{-4}	1.75×10^{-3}	9.35×10^{-3}
6.5	18.625	−0.924	0.026	−0.337	5.55×10^{-4}	2.66×10^{-3}	0.0142
7.0	15.066	−0.894	0.021	−0.327	7.72×10^{-4}	3.74×10^{-3}	0.0200
7.5	12.223	−0.866	0.017	−0.318	1.03×10^{-3}	1.03×10^{-3}	0.0267
8.0	10.051	−0.840	0.014	−0.310	1.29×10^{-3}	6.31×10^{-3}	0.0337
8.5	8.282	−0.816	0.012	−0.302	1.59×10^{-3}	7.73×10^{-3}	0.0413
9.0	7.028	−0.795	0.010	−0.295	1.83×10^{-3}	8.92×10^{-3}	0.0476
9.5	6.267	−0.780	8.33×10^{-3}	−0.289	1.98×10^{-3}	9.62×10^{-3}	0.0514
10.0	5.426	−0.763	7.30×10^{-3}	−0.284	2.23×10^{-3}	0.0108	0.0578
10.5	5.180	−0.755	6.39×10^{-3}	−0.278	2.21×10^{-3}	0.0107	0.0573
11.0	5.214	−0.753	5.83×10^{-3}	−0.275	2.08×10^{-3}	0.0101	0.0539
11.5	7.094	−0.778	5.44×10^{-3}	−0.272	1.07×10^{-3}	4.60×10^{-3}	0.0275
12.0	4.841	−0.744	5.35×10^{-3}	−0.272	2.20×10^{-3}	0.0107	0.0572
12.5	3.040	−0.716	7.01×10^{-3}	−0.282	4.01×10^{-3}	0.0191	0.1020
13.0	0.827	−0.621	0.012	−0.302	6.82×10^{-3}	0.0317	0.1690
13.5	2.775	−0.701	5.73×10^{-3}	−0.275	4.01×10^{-3}	0.0191	0.1022
14.0	2.445	−0.683	4.39×10^{-3}	−0.265	4.09×10^{-3}	0.0195	0.1042

Table C.4: The fitting results for the MP2 *ab initio* dipole moments of the CO_2 dimer using the ACCT basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	35.367	-1.018	0.0471	-0.314	1.17×10^{-4}	2.43×10^{-4}	0.0295
5.0	27.468	-0.977	0.0331	-0.298	1.24×10^{-4}	4.52×10^{-4}	0.0223
5.5	21.584	-0.939	0.0240	-0.284	2.18×10^{-4}	9.72×10^{-4}	0.0170
6.0	17.102	-0.904	0.0179	-0.271	3.71×10^{-4}	1.74×10^{-3}	0.0133
6.5	13.549	-0.871	0.0138	-0.259	5.83×10^{-4}	2.79×10^{-3}	0.0160
7.0	10.731	-0.839	0.0109	-0.249	8.49×10^{-4}	4.12×10^{-3}	0.0236
7.5	8.453	-0.807	8.74×10^{-3}	-0.240	1.18×10^{-3}	5.72×10^{-3}	0.0328
8.0	6.741	-0.779	7.13×10^{-3}	-0.231	1.52×10^{-3}	7.38×10^{-3}	0.0423
8.5	5.458	-0.752	5.90×10^{-3}	-0.224	1.85×10^{-3}	9.01×10^{-3}	0.0517
9.0	4.496	-0.729	4.95×10^{-3}	-0.216	2.17×10^{-3}	0.0106	0.0605
9.5	3.829	-0.709	4.19×10^{-3}	-0.210	2.43×10^{-3}	0.0118	0.0676
10.0	3.228	-0.689	3.61×10^{-3}	-0.204	2.74×10^{-3}	0.0133	0.0760
10.5	2.850	-0.674	3.11×10^{-3}	-0.198	2.93×10^{-3}	0.0142	0.0812
11.0	2.617	-0.663	2.73×10^{-3}	-0.193	3.03×10^{-3}	0.0147	0.0841
11.5	2.336	-0.650	2.45×10^{-3}	-0.189	3.24×10^{-3}	0.0156	0.0895
12.0	2.597	-0.656	2.17×10^{-3}	-0.184	2.78×10^{-3}	0.0134	0.0770
12.5	2.701	-0.657	2.08×10^{-3}	-0.183	2.59×10^{-3}	0.0125	0.0717
13.0	1.824	-0.623	1.96×10^{-3}	-0.180	3.71×10^{-3}	0.0178	0.1023
13.5	1.398	-0.590	1.30×10^{-3}	-0.166	4.03×10^{-3}	0.0194	0.1110
14.0	1.152	-0.573	1.21×10^{-3}	-0.163	4.51×10^{-3}	0.0216	0.1236

Table C.5: The fitting results for the CCSD *ab initio* dipole moments of the CO_2 dimer using the ACCT basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	149.618	-1.250	0.074	-0.380	1.76×10^{-4}	7.04×10^{-4}	0.0123
5.0	103.070	-1.192	0.057	-0.368	7.83×10^{-5}	2.74×10^{-4}	8.67×10^{-3}
5.5	57.239	-1.108	0.046	-0.359	3.60×10^{-4}	1.72×10^{-3}	9.85×10^{-3}
6.0	33.343	-1.034	0.039	-0.350	8.26×10^{-4}	4.00×10^{-3}	0.0229
6.5	30.081	-1.015	0.033	-0.343	7.86×10^{-4}	3.79×10^{-3}	0.0217
7.0	16.980	-0.944	0.029	-0.338	1.54×10^{-3}	7.49×10^{-3}	0.0429
7.5	7.869	-0.851	0.025	-0.332	2.58×10^{-3}	0.0125	0.0716
8.0	4.071	-0.771	0.021	-0.324	3.39×10^{-3}	0.0164	0.0936
8.5	2.433	-0.708	0.016	-0.312	3.96×10^{-3}	0.0191	0.1092
9.0	1.750	-0.665	0.011	-0.298	4.28×10^{-3}	0.0206	0.1177
9.5	1.445	-0.638	7.19×10^{-3}	-0.281	4.42×10^{-3}	0.0213	0.1216
10.0	1.293	-0.621	4.59×10^{-3}	-0.263	4.47×10^{-3}	0.0215	0.1229
10.5	1.200	-0.608	2.86×10^{-3}	-0.245	4.48×10^{-3}	0.0215	0.1232
11.0	1.115	-0.596	1.72×10^{-3}	-0.225	4.50×10^{-3}	0.0217	0.1239
11.5	1.013	-0.584	9.66×10^{-4}	-0.203	4.58×10^{-3}	0.0220	0.1260
12.0	0.887	-0.568	4.72×10^{-4}	-0.176	4.73×10^{-3}	0.0227	0.1300
12.5	0.748	-0.549	1.77×10^{-4}	-0.139	4.95×10^{-3}	0.0238	0.1359
13.0	0.612	-0.528	3.94×10^{-5}	-0.084	5.23×10^{-3}	0.0250	0.1432
13.5	0.489	-0.507	3.15×10^{-6}	0.009	5.54×10^{-3}	0.0265	0.1514
14.0	0.391	-0.486	2.30×10^{-8}	0.186	5.86×10^{-3}	0.0279	0.1597

Table C.6: The fitting results for the CCSD(T) *ab initio* dipole moments of the CO_2 dimer using the ACCT basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	160.865	−1.259	0.094	−0.402	2.09×10^{-4}	8.42×10^{-4}	0.0128
5.0	120.550	−1.212	0.072	−0.391	1.57×10^{-4}	6.43×10^{-4}	7.43×10^{-3}
5.5	72.226	−1.138	0.059	−0.382	2.15×10^{-4}	9.80×10^{-4}	5.67×10^{-3}
6.0	43.505	−1.068	0.050	−0.374	6.52×10^{-4}	3.14×10^{-3}	0.0182
6.5	43.018	−1.061	0.043	−0.368	4.73×10^{-4}	2.25×10^{-3}	0.0130
7.0	22.338	−0.980	0.039	−0.364	1.41×10^{-3}	6.85×10^{-3}	0.0396
7.5	9.091	−0.872	0.035	−0.359	2.68×10^{-3}	0.0129	0.0748
8.0	4.265	−0.780	0.028	−0.350	3.60×10^{-3}	0.0173	0.1003
8.5	2.420	−0.710	0.021	−0.337	4.22×10^{-3}	0.0203	0.1172
9.0	1.705	−0.663	0.014	−0.320	4.54×10^{-3}	0.0218	0.1260
9.5	1.396	−0.634	8.36×10^{-3}	−0.301	4.68×10^{-3}	0.0225	0.1300
10.0	1.244	−0.616	4.74×10^{-3}	−0.278	4.73×10^{-3}	0.0227	0.1313
10.5	1.150	−0.602	2.50×10^{-3}	−0.253	4.75×10^{-3}	0.0228	0.1318
11.0	1.067	−0.591	1.20×10^{-3}	−0.225	4.77×10^{-3}	0.0229	0.1325
11.5	0.972	−0.578	5.01×10^{-4}	−0.191	4.85×10^{-3}	0.0233	0.1345
12.0	0.865	−0.564	1.62×10^{-4}	−0.149	4.98×10^{-3}	0.0239	0.1380
12.5	0.755	−0.550	3.50×10^{-5}	−0.091	5.15×10^{-3}	0.0247	0.1428
13.0	0.659	−0.536	3.79×10^{-6}	−0.009	5.34×10^{-3}	0.0256	0.1478
13.5	0.615	−0.528	1.51×10^{-7}	0.108	5.41×10^{-3}	0.0259	0.1498
14.0	0.535	−0.515	3.71×10^{-9}	0.242	5.65×10^{-3}	0.0270	0.1559

Table C.7: The fitting results for the RHF *ab initio* dipole moments of the CO_2 dimer using the ACCQ basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	49.069	−1.074	0.081	−0.389	7.86×10^{-5}	1.66×10^{-4}	0.0154
5.0	38.863	−1.034	0.057	−0.373	9.07×10^{-5}	3.44×10^{-4}	0.0112
5.5	30.762	−0.997	0.042	−0.359	1.80×10^{-4}	8.09×10^{-4}	7.99×10^{-3}
6.0	24.256	−0.961	0.031	−0.347	3.34×10^{-4}	1.58×10^{-3}	8.44×10^{-3}
6.5	19.132	−0.927	0.024	−0.335	5.47×10^{-4}	2.64×10^{-3}	0.0141
7.0	15.202	−0.896	0.019	−0.325	7.99×10^{-4}	3.88×10^{-3}	0.0207
7.5	12.242	−0.867	0.015	−0.315	1.07×10^{-3}	5.22×10^{-3}	0.0278
8.0	10.115	−0.842	0.003	−0.254	1.33×10^{-3}	6.47×10^{-3}	0.0345
8.5	8.203	−0.815	0.010	−0.299	1.66×10^{-3}	8.08×10^{-3}	0.0431
9.0	7.117	−0.797	8.45×10^{-3}	−0.291	1.85×10^{-3}	8.99×10^{-3}	0.0479
9.5	5.918	−0.775	7.23×10^{-3}	−0.285	2.18×10^{-3}	0.0106	0.0564
10.0	4.958	−0.754	6.12×10^{-3}	−0.278	2.49×10^{-3}	0.0121	0.0643
10.5	5.092	−0.753	5.21×10^{-3}	−0.272	2.26×10^{-3}	0.0110	0.0586
11.0	4.193	−0.733	4.80×10^{-3}	−0.269	2.72×10^{-3}	0.0132	0.0703
11.5	3.127	−0.703	4.05×10^{-3}	−0.262	3.36×10^{-3}	0.0162	0.0863
12.0	2.631	−0.683	3.28×10^{-3}	−0.254	3.63×10^{-3}	0.0175	0.0932
12.5	1.834	−0.649	2.75×10^{-3}	−0.248	4.44×10^{-3}	0.0212	0.1129
13.0	1.356	−0.613	1.42×10^{-3}	−0.223	4.82×10^{-3}	0.0229	0.1223
13.5	1.040	−0.586	9.12×10^{-4}	−0.207	5.28×10^{-3}	0.0250	0.1336
14.0	0.854	−0.615	6.28×10^{-3}	−0.277	6.70×10^{-3}	0.0311	0.1660

Table C.8: The fitting results for the MP2 *ab initio* dipole moments of the CO_2 dimer using the ACCQ basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	36.554	−1.023	0.045	−0.313	1.12×10^{-4}	2.37×10^{-4}	0.0295
5.0	29.352	−0.986	0.031	−0.297	9.01×10^{-5}	2.63×10^{-4}	0.0219
5.5	23.197	−0.949	0.023	−0.282	1.72×10^{-4}	7.59×10^{-4}	0.0171
6.0	18.040	−0.911	0.017	−0.269	3.51×10^{-4}	1.66×10^{-3}	0.0131
6.5	13.990	−0.876	0.013	−0.258	6.00×10^{-4}	2.90×10^{-3}	0.0166
7.0	10.932	−0.842	0.010	−0.247	8.93×10^{-4}	4.34×10^{-3}	0.0249
7.5	8.634	−0.811	8.19×10^{-3}	−0.238	1.21×10^{-3}	5.91×10^{-3}	0.0339
8.0	6.964	−0.784	6.68×10^{-3}	−0.229	1.53×10^{-3}	7.45×10^{-3}	0.0427
8.5	5.575	−0.756	5.55×10^{-3}	−0.222	1.90×10^{-3}	9.22×10^{-3}	0.0529
9.0	4.709	−0.735	4.65×10^{-3}	−0.214	2.16×10^{-3}	0.0105	0.0600
9.5	3.909	−0.713	3.99×10^{-3}	−0.208	2.49×10^{-3}	0.0121	0.0691
10.0	3.261	−0.692	3.42×10^{-3}	−0.202	2.82×10^{-3}	0.0136	0.0781
10.5	3.016	−0.681	2.95×10^{-3}	−0.196	2.88×10^{-3}	0.0139	0.0798
11.0	2.515	−0.662	2.66×10^{-3}	−0.192	3.27×10^{-3}	0.0157	0.0903
11.5	2.148	−0.644	2.28×10^{-3}	−0.187	3.54×10^{-3}	0.0170	0.0977
12.0	1.939	−0.632	2.01×10^{-3}	−0.182	3.69×10^{-3}	0.0177	0.1017
12.5	1.604	−0.613	1.78×10^{-3}	−0.177	4.09×10^{-3}	0.0196	0.1123
13.0	1.288	−0.589	1.45×10^{-3}	−0.170	4.49×10^{-3}	0.0214	0.1229
13.5	1.020	−0.565	1.13×10^{-3}	−0.161	4.91×10^{-3}	0.0233	0.1338
14.0	1.473	−0.609	1.86×10^{-3}	−0.179	4.45×10^{-3}	0.0212	0.1216

Table C.9: The fitting results for the RHF *ab initio* dipole moments of the CO_2 dimer using the APC3 basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	48.415	−1.072	0.082	−0.390	7.97×10^{-5}	1.67×10^{-4}	0.0152
5.0	38.585	−1.033	0.058	−0.374	8.82×10^{-5}	3.28×10^{-4}	0.0109
5.5	30.746	−0.997	0.042	−0.360	1.70×10^{-4}	7.59×10^{-4}	7.93×10^{-3}
6.0	24.260	−0.961	0.032	−0.348	3.24×10^{-4}	1.53×10^{-3}	8.15×10^{-3}
6.5	19.079	−0.927	0.025	−0.336	5.40×10^{-4}	2.61×10^{-3}	0.0139
7.0	15.059	−0.894	0.019	−0.326	8.04×10^{-4}	3.91×10^{-3}	0.0209
7.5	12.017	−0.864	0.015	−0.316	1.09×10^{-3}	5.33×10^{-3}	0.0284
8.0	9.712	−0.837	0.012	−0.307	1.39×10^{-3}	6.80×10^{-3}	0.0363
8.5	7.972	−0.812	0.010	−0.299	1.69×10^{-3}	8.24×10^{-3}	0.0440
9.0	6.650	−0.789	8.37×10^{-3}	−0.291	1.98×10^{-3}	9.62×10^{-3}	0.0513
9.5	5.622	−0.769	6.99×10^{-3}	−0.284	2.25×10^{-3}	0.0109	0.0583
10.0	4.965	−0.753	5.88×10^{-3}	−0.277	2.43×10^{-3}	0.0118	0.0628
10.5	4.511	−0.741	5.06×10^{-3}	−0.271	2.55×10^{-3}	0.0124	0.0660
11.0	3.780	−0.722	4.43×10^{-3}	−0.266	2.91×10^{-3}	0.0141	0.0751
11.5	3.638	−0.715	3.72×10^{-3}	−0.260	2.86×10^{-3}	0.0138	0.0737
12.0	3.721	−0.714	3.38×10^{-3}	−0.256	2.69×10^{-3}	0.0130	0.0695
12.5	3.749	−0.712	3.11×10^{-3}	−0.253	2.56×10^{-3}	0.0124	0.0662
13.0	2.674	−0.682	2.88×10^{-3}	−0.250	3.50×10^{-3}	0.0168	0.0898
13.5	1.769	−0.663	4.61×10^{-3}	−0.267	5.08×10^{-3}	0.0240	0.1279
14.0	0.345	−0.541	0.035	−0.340	7.17×10^{-3}	0.0334	0.1782

Table C.10: The fitting results for the MP2 *ab initio* dipole moments of the CO_2 dimer using the APC3 basis set.

Breakpoint (Å)	a	b	c	d	RMSE	Maximum Error	Relative Error
4.5	35.520	−1.020	0.045	−0.313	1.14×10^{-4}	2.38×10^{-4}	0.0291
5.0	28.457	−0.982	0.032	−0.297	9.79×10^{-5}	3.06×10^{-4}	0.0217
5.5	22.652	−0.946	0.023	−0.283	1.74×10^{-4}	7.61×10^{-4}	0.0167
6.0	17.746	−0.910	0.017	−0.270	3.42×10^{-4}	1.61×10^{-3}	0.0128
6.5	13.785	−0.874	0.013	−0.258	5.86×10^{-4}	2.83×10^{-3}	0.0163
7.0	10.763	−0.841	0.010	−0.248	8.79×10^{-4}	4.27×10^{-3}	0.0246
7.5	8.483	−0.809	8.15×10^{-3}	−0.238	1.20×10^{-3}	5.85×10^{-3}	0.0337
8.0	6.772	−0.781	6.63×10^{-3}	−0.229	1.54×10^{-3}	7.49×10^{-3}	0.0430
8.5	5.431	−0.754	5.47×10^{-3}	−0.222	1.90×10^{-3}	9.22×10^{-3}	0.0530
9.0	4.456	−0.729	4.56×10^{-3}	−0.214	2.22×10^{-3}	0.0108	0.0620
9.5	3.696	−0.707	3.85×10^{-3}	−0.207	2.54×10^{-3}	0.0123	0.0708
10.0	3.112	−0.687	3.27×10^{-3}	−0.201	2.84×10^{-3}	0.0137	0.0790
10.5	2.660	−0.669	2.80×10^{-3}	−0.195	3.11×10^{-3}	0.0150	0.0863
11.0	2.251	−0.650	2.41×10^{-3}	−0.189	3.42×10^{-3}	0.0165	0.0946
11.5	1.968	−0.635	2.05×10^{-3}	−0.183	3.63×10^{-3}	0.0175	0.1004
12.0	1.846	−0.626	1.77×10^{-3}	−0.177	3.67×10^{-3}	0.0177	0.1015
12.5	1.763	−0.619	1.57×10^{-3}	−0.173	3.69×10^{-3}	0.0177	0.1019
13.0	1.772	−0.616	1.39×10^{-3}	−0.168	3.55×10^{-3}	0.0171	0.0982
13.5	2.220	−0.631	1.27×10^{-3}	−0.165	2.72×10^{-3}	0.0131	0.0753
14.0	1.925	−0.621	1.31×10^{-3}	−0.166	3.21×10^{-3}	0.0155	0.0891

C.3 Fitting Residuals

Table C.11: The difference between the ACCT *ab initio* dipole moments and the dipole moments calculated from the fitting equation at the breakpoint with the lowest root mean squared error, which was at 4.5 Å for RHF and MP2 and 5.0 Å for CCSD and CCSD(T).

C-C Distance		ACCT			
Å	au	RHF	MP2	CCSD	CCSD(T)
3.5	6.614 041 439	0.000 198 603	0.000 166 453	−0.000 222 323	−0.000 642 911
4.0	7.558 904 502	−0.000 142 895	−0.000 126 417	0.000 273 856	0.000 405 83
4.5	8.503 767 565	$2.608\,56 \times 10^{-5}$	$2.428\,95 \times 10^{-5}$	−0.000 104 017	$-5.693\,03 \times 10^{-5}$
5.0	9.448 630 627	$-4.606\,02 \times 10^{-5}$	$-7.110\,79 \times 10^{-5}$	$1.334\,85 \times 10^{-5}$	$-1.319\,23 \times 10^{-6}$
5.5	10.393 493 69	−0.000 124 917	−0.000 178 023	$5.396\,15 \times 10^{-5}$	$2.358\,72 \times 10^{-5}$
6.0	11.338 356 75	−0.000 163 66	−0.000 236 615	$7.693\,01 \times 10^{-6}$	$-9.684\,28 \times 10^{-6}$
6.5	12.283 219 82	−0.000 162 113	−0.000 243 355	$-7.983\,03 \times 10^{-5}$	$-8.516\,89 \times 10^{-5}$
7.0	13.228 082 88	−0.000 139 564	−0.000 220 166	$-3.813\,84 \times 10^{-5}$	$-3.236\,64 \times 10^{-5}$
7.5	14.172 945 94	−0.000 109 883	−0.000 183 275	$-1.057\,84 \times 10^{-5}$	$3.882\,13 \times 10^{-8}$
8.0	15.117 809	$-8.239\,48 \times 10^{-5}$	−0.000 146 501	$-7.513\,47 \times 10^{-6}$	$3.512\,28 \times 10^{-6}$
8.5	16.062 672 07	$-5.874\,82 \times 10^{-5}$	−0.000 112 61	$-7.169\,82 \times 10^{-6}$	$2.215\,08 \times 10^{-6}$
9.0	17.007 535 13	$-4.110\,21 \times 10^{-5}$	$-8.377\,48 \times 10^{-5}$	$-1.242\,61 \times 10^{-5}$	$-5.170\,73 \times 10^{-6}$
9.5	17.952 398 19	$-2.799\,06 \times 10^{-5}$	$-6.080\,72 \times 10^{-5}$	$-1.434\,89 \times 10^{-5}$	$-9.038\,62 \times 10^{-6}$
10.0	18.897 261 25	$-1.766\,48 \times 10^{-5}$	$-4.162\,32 \times 10^{-5}$	$-1.329\,44 \times 10^{-5}$	$-9.602\,99 \times 10^{-6}$
10.5	19.842 124 32	$-1.129\,27 \times 10^{-5}$	$-2.813\,16 \times 10^{-5}$	$-1.071\,01 \times 10^{-5}$	$-8.277\,04 \times 10^{-6}$
11.0	20.786 987 38	-6.48×10^{-6}	$-1.759\,21 \times 10^{-5}$	$-7.797\,17 \times 10^{-6}$	$-6.319\,09 \times 10^{-6}$
11.5	21.731 850 44	$-3.404\,61 \times 10^{-6}$	$-9.536\,86 \times 10^{-6}$	$-5.188\,03 \times 10^{-6}$	$-4.406\,21 \times 10^{-6}$
12.0	22.676 713 51	$-1.769\,56 \times 10^{-6}$	$-4.541\,01 \times 10^{-6}$	-3.1749×10^{-6}	$-2.927\,17 \times 10^{-6}$
12.5	23.621 576 57	$-2.273\,77 \times 10^{-7}$	$-2.695\,34 \times 10^{-7}$	$-1.734\,15 \times 10^{-6}$	-1.836×10^{-6}
13.0	24.566 439 63	$1.657\,87 \times 10^{-6}$	$2.921\,95 \times 10^{-6}$	$-7.813\,93 \times 10^{-7}$	$-1.122\,17 \times 10^{-6}$
13.5	25.511 302 69	1.0756×10^{-6}	$3.516\,07 \times 10^{-6}$	$-1.641\,04 \times 10^{-7}$	$-6.610\,39 \times 10^{-7}$
14.0	26.456 165 76	$1.189\,45 \times 10^{-6}$	$4.871\,75 \times 10^{-6}$	$2.395\,78 \times 10^{-7}$	$-3.779\,44 \times 10^{-7}$
14.5	27.401 028 82	$9.111\,21 \times 10^{-7}$	$4.964\,47 \times 10^{-6}$	$4.580\,33 \times 10^{-7}$	$2.083\,97 \times 10^{-6}$
15.0	28.345 891 88	$1.085\,17 \times 10^{-6}$	$5.708\,85 \times 10^{-6}$	$3.459\,67 \times 10^{-6}$	$1.980\,22 \times 10^{-6}$

Table C.12: The difference between the *ab initio* dipole moments and the dipole moments calculated from the fitting equation at the breakpoint with the lowest root mean squared error for the ACCQ and APC3 basis sets. The RHF breakpoint was 4.5 Å and the MP2 was 5.0 Å for both basis sets.

C-C Distance		ACCQ		APC3	
Å	au	RHF	MP2	RHF	MP2
3.5	6.614 041 439	0.000 136 738	0.000 263 082	0.000 142 34	0.000 305 707
4.0	7.558 904 502	$-9.867\,22 \times 10^{-5}$	−0.000 185 426	−0.000 102 863	−0.000 211 986
4.5	8.503 767 565	$1.798\,17 \times 10^{-5}$	2.4798×10^{-5}	$1.878\,08 \times 10^{-5}$	$2.589\,03 \times 10^{-5}$
5.0	9.448 630 627	$-7.176\,28 \times 10^{-5}$	$3.149\,52 \times 10^{-6}$	$-7.663\,08 \times 10^{-5}$	$4.306\,01 \times 10^{-6}$
5.5	10.393 493 69	−0.000 140 532	$-5.426\,98 \times 10^{-5}$	−0.000 145 592	$-5.811\,73 \times 10^{-5}$
6.0	11.338 356 75	−0.000 165 532	−0.000 102 519	−0.000 167 07	−0.000 106 068
6.5	12.283 219 82	−0.000 158 184	−0.000 128 904	−0.000 157 76	−0.000 129 674
7.0	13.228 082 88	−0.000 134 909	−0.000 133 7	−0.000 133 558	−0.000 133 248
7.5	14.172 945 94	−0.000 106 98	−0.000 123 151	−0.000 105 536	−0.000 122 336
8.0	15.117 809	$-8.100\,68 \times 10^{-5}$	−0.000 105 91	$-7.916\,64 \times 10^{-5}$	−0.000 104 361
8.5	16.062 672 07	$-5.710\,58 \times 10^{-5}$	$-8.407\,14 \times 10^{-5}$	$-5.711\,95 \times 10^{-5}$	$-8.372\,65 \times 10^{-5}$
9.0	17.007 535 13	$-4.094\,64 \times 10^{-5}$	$-6.688\,17 \times 10^{-5}$	$-3.983\,76 \times 10^{-5}$	$-6.532\,94 \times 10^{-5}$
9.5	17.952 398 19	$-2.661\,86 \times 10^{-5}$	$-4.868\,92 \times 10^{-5}$	$-2.684\,97 \times 10^{-5}$	$-4.862\,64 \times 10^{-5}$
10.0	18.897 261 25	$-1.729\,95 \times 10^{-5}$	$-3.483\,85 \times 10^{-5}$	$-1.775\,62 \times 10^{-5}$	$-3.503\,09 \times 10^{-5}$
10.5	19.842 124 32	$-1.155\,45 \times 10^{-5}$	$-2.494\,59 \times 10^{-5}$	$-1.109\,72 \times 10^{-5}$	$-2.416\,59 \times 10^{-5}$
11.0	20.786 987 38	$-5.915\,18 \times 10^{-6}$	$-1.493\,64 \times 10^{-5}$	-6.1455×10^{-6}	$-1.550\,45 \times 10^{-5}$
11.5	21.731 850 44	$-2.997\,07 \times 10^{-6}$	$-9.122\,18 \times 10^{-6}$	$-3.540\,01 \times 10^{-6}$	$-9.430\,05 \times 10^{-6}$
12.0	22.676 713 51	$-1.379\,13 \times 10^{-6}$	$-4.466\,43 \times 10^{-6}$	$-1.462\,34 \times 10^{-6}$	$-4.879\,78 \times 10^{-6}$
12.5	23.621 576 57	$2.480\,34 \times 10^{-7}$	$-8.263\,34 \times 10^{-7}$	$-1.716\,76 \times 10^{-7}$	$-1.325\,09 \times 10^{-6}$
13.0	24.566 439 63	$3.254\,72 \times 10^{-7}$	$1.282\,66 \times 10^{-6}$	$3.482\,76 \times 10^{-7}$	$1.111\,26 \times 10^{-6}$
13.5	25.511 302 69	$3.516\,81 \times 10^{-7}$	2.2029×10^{-6}	$8.085\,46 \times 10^{-7}$	$2.766\,07 \times 10^{-6}$
14.0	26.456 165 76	$1.506\,01 \times 10^{-6}$	$4.430\,15 \times 10^{-6}$	$1.606\,57 \times 10^{-6}$	$4.165\,25 \times 10^{-6}$
14.5	27.401 028 82	$1.116\,88 \times 10^{-6}$	$4.315\,57 \times 10^{-6}$	$1.250\,61 \times 10^{-6}$	$4.411\,61 \times 10^{-6}$
15.0	28.345 891 88	$1.203\,41 \times 10^{-6}$	$4.919\,07 \times 10^{-6}$	$9.713\,95 \times 10^{-7}$	$4.990\,17 \times 10^{-6}$

Vita

Randi Beil graduated from Mary Baldwin College (now Mary Baldwin University) in May 2014 with a BS in Chemistry with Honors and a concentration in Material Chemistry, a BS in Mathematics, and a minor in Physics. She began at the University of Tennessee, Knoxville in the Fall of 2014 and has spent her time studying the properties of carbon dioxide. She has presented her research at the National Meeting of the American Chemical Society (ACS), the Southeast Regional Meeting of the ACS (SERMACS), and the Southeast Theoretical Chemistry Association (SETCA). She received the Keenan Teaching Award in 2016 and 2018. In the 2018-2019 academic year, she served as the philanthropy chair for the Association of Chemistry Graduate Students (ACGS).