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Computational Studies of the N2-H2 Interaction-Induced Dipole Moment

Hailey R. Bureau
hailey.bureau@gmail.com

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Hailey R. Bureau
Department of Chemistry
Chancellor's Honors Program
The University of Tennessee, Knoxville

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TABLE OF CONTENTS

INTRODUCTION

INFRARED SPECTROSCOPY

Infrared spectroscopy is a technique used extensively in the field of organic chemistry to identify unknown molecules by recording the absorption spectrum of the molecule's infrared-active vibrational modes. The vibrational mode of a molecule is only infrared active if the molecule has a dipole moment that changes during the vibration. However, if a dipole can be induced "at the molecular rotovibrational frequencies of the colliding molecules and emit/absorb radiation"[1] a collision-induced infrared absorption spectrum can also result from a molecule's normally inactive vibrational mode.

DIPOLES

Dipole moments measure the degree of polarity of a molecule. Both H_2 and N_2 are nonpolar molecules due to their symmetry and are categorized in the $D_{\infty h}$ point group. Therefore, they have zero dipole moments and the vibrational motions of isolated H_2 and N_2 would not appear in an infrared absorption spectrum. However, dipole moments can be created by collisional interactions, which induce transient electric dipole moments by multipolar induction and exchange and dispersion forces, which are the same mechanisms that generate the intermolecular forces.[1] Three important factors to consider in evaluating net dipole moments for a molecular pair are the molecular geometry, the amount of charge, and the distance, R, between the molecules. Studies of weakly bound dimers yield information about the redistribution of electron density that occurs during dimer formation and about the inception of intermolecular forces. "These interaction-induced electrical properties provide a starting point for computations of collision-

induced absorption line shapes and for the analysis of collision-induced light scattering phenomena".[2]

COLLISION-INDUCED ABSORPTION

The phenomenon of induced dipoles from collisions resulting in the infrared emission and absorption of radiation is referred to as Collision-Induced Absorption (CIA). Some of the earliest detailed studies of CIA were conducted by Welsh and associates in 1949.[3, 4] "Collision between H_2 molecules yield CIA, consisting of roto-translational and roto-vibrational bands, with peaks located in far-red and infrared spectral regions".[5] This is an interesting molecular interaction because even gases which are usually infrared inactive, such as N_2 and H_2, will begin to absorb radiation if collision densities are high enough.[1] This type of absorption is a result of "transient intermolecular complexes of two colliding molecules in which dipoles are induced by molecular interactions".[6] CIA has been applied to the field of astrochemistry to study the atmospheres of giant planets and their moons, which are rich in H_2. It is a supramolecular process that has been studied in great detail in various dense gases, especially in hydrogen and mixtures of hydrogen and helium.[6] These collision-induced absorption events are the only way that H_2 molecules in these planets' atmospheres can effectively absorb infrared radiation from the Sun. Because the molecules' bond lengths are not fixed it is necessary to understand the role that molecular vibrations play in the N_2 and H_2 dipole moment to develop better models of atmospheric opacity. Opacity is the measure of how much radiation can pass through an object, but in this case opacity describes radiation passing through atmospheric molecules.[7]

APPLICATIONS

In the case of Titan, one of the largest moons of Saturn, its atmosphere consists predominantly of N_2, He, and H_2 with smaller, though significant, amounts of CH_4 present. From the findings of Birnbaum et al. who studied the CIA of $(H_2)_2$ and H_2-He, "H_2 and He are the only well-mixed constituents of substantial abundance in all the giant planets. As such, the spectral variation of their absorption can be used to sense temperature profiles at atmospheric pressures …using ground-based measurements or using spacecraft infrared instruments".[6] The amount of H_2 is a result of the production of more complex carbon species from methane. Some of the H_2 moves into the troposphere where it conspires to act as a "partial thermal blanket, enhancing Titan's greenhouse".[8] The troposphere is the lowest portion of a planet's atmosphere and contains virtually all of the water vapor and aerosols present in the atmosphere and accounts for most of the atmosphere's mass.[7] CIA is very common in high-density gases; the troposphere is "dense enough to provide most of the infrared opacity through CIA".[8] The opacities due to collision-induced absorption depend on the abundances of H_2, N_2, and CH_4 available in the troposphere. This is responsible for the weak greenhouse effect that raises Titan's surface temperature. Understanding Titan's atmosphere is very important because although Titan's atmosphere is unlike Earth's now, it has the closest atmosphere to what Earth's atmosphere was 4 billion years ago, when nucleic acid molecules that led to the development of life first combined.[7] Birnbaum et al.[6] also described the importance of $(H_2)_2$ and H_2-He CIA events because they are the primary mechanism for radiative cooling of the tropospheres and lower stratospheres of the giant planets. Their distinct

absorption bands have also been used extensively for determining the relative abundances of H_2 and He present in the atmospheres by modeling the differences in the spectral shapes of $(H_2)_2$ and H_2-He or by matching the results of infrared and radio occultation techniques to give an accurate measurement of molecular weight.[6]

This research may lead to a better understanding of the intermolecular forces at work in long-range induction of a quadrupole. Understanding the way the dipole moment changes with H_2 bond length is important because the variation in dipole moment with H_2 bond length would allow H_2 molecules to absorb infrared radiation at the moment they are colliding with N_2, giving rise to the CIA phenomenon. Interpreting the CIA events of molecules has proved to be an extremely useful tool in the field of astrochemistry for understanding the molecular properties of the atmospheres of giant planets. Studies of interaction-induced dipoles provide data about the redistribution of electron density during dimer formation and further understanding of the principles of intermolecular forces.

METHODS

Chemical Methods

APPLIED ELECTRIC FIELD

Another important aspect of dipole moment calculations is the response of the system to an external electric field. An electric field is the force per unit charge experienced by a test charge in the vicinity of one or more finite charges. This affects the molecular polarizability, which means that a positive-negative charge displacement has occurred throughout the molecule leading to an induced surface charge. The following equation[9] relates the energy of a molecule to a weak external electric field:

$$E(\vec{F}) = E(\vec{F}=0) - \vec{\mu}_0 \cdot \vec{F} - \frac{1}{2}\sum_{i=x,y,z}\sum_{j=x,y,z}\alpha_{ij}F_iF_j \qquad (1)$$

In Eqn. 1, the energy, E, of a molecule is the response of the molecule to an external electric field F, where F_x, F_y, and F_z are the components of the field. The molecule's dipole moment is accounted for by the term μ_0 and α is a 3 x 3 matrix representing the polarizability.[9] For stronger fields, Eqn. 1 can be extended as follows[9]:

$$\begin{aligned} W &= \left\langle \Psi \middle| \hat{H} \middle| \Psi \right\rangle \\ &= W^{(0)} - \mu_\alpha^{(0)}F_\alpha - \frac{1}{2}\alpha_{\alpha\beta}F_\alpha F_\beta - \frac{1}{6}\beta_{\alpha\beta\gamma}F_\alpha F_\beta F_\gamma - \frac{1}{24}\gamma_{\alpha\beta\gamma\delta}F_\alpha F_\beta F_\gamma F_\delta \\ &\quad - \frac{1}{3}\Theta_{\alpha\beta}^{(0)}F_{\alpha\beta} - \frac{1}{3}A_{\gamma,\alpha\beta}F_\gamma F_{\alpha\beta} - \frac{1}{6}\beta_{\alpha\beta,\gamma\delta}F_\alpha F_\beta F_{\gamma_\delta} - \frac{1}{6}C_{\alpha\beta,\gamma\delta}F_{\alpha\beta}F_{\gamma\delta} - \ldots \end{aligned} \qquad (2)$$

From these equations, it is possible to calculate the induced dipole moment, the topic of interest. In these calculations, the applied field is uniform and constant for every calculation.

Mathematical Methods

Previous studies of the $(H_2)_2$ van der Waals dimer have been conducted by Burton and Senff[10] and by Kohler and Schaefer.[11] In this study, coupled cluster *ab initio* calculations of the interaction-induced dipole moment of a similar dimer, the N_2-H_2 van der Waals dimer have been analyzed. The atom-centered aug-cc-pVTZ basis sets for hydrogen and nitrogen were used to carry out these calculations using the CCSD approach described below. Large, flexible basis sets, which include p, d, etc. orbitals, are used to account for the electron correlation, which is neglected when using the standard orbitals for H_2 and N_2. Initially, five specific orientations of the N_2-H_2 interaction were

analyzed: linear, T-shaped with N_2 horizontal, T-shaped with H_2 horizontal, crossed, and parallel described in Table 1 below. Using fixed orientations of the molecules in a defined coordinate system, Fig. 1, is necessary to arrive at reasonable conclusions because of the potential spatial rotation of the molecules.[12]

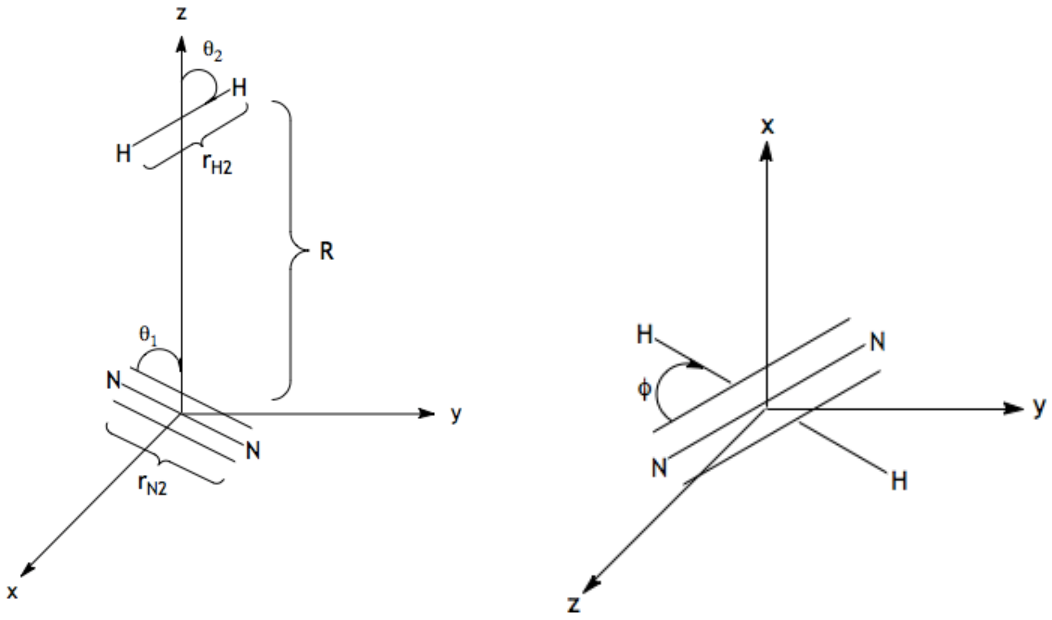

Figure 1: Example orientation of the molecules with angle assignments shown. The value R is the center-of-mass distance between the molecules and the value r represents the N_2 and H_2 monomer bond lengths.

Configuration	Φ (deg)	Θ_1 (deg)	Θ_2 (deg)
Linear	0	0	0
T-Shaped 1	0	0	90
T-Shaped 2	0	90	0
Parallel	0	90	90
Crossed	90	90	90
A	0	45	0
B	0	0	45
C	0	45	45
D	0	45	90
E	0	90	45
F	0	45	45
G	90	45	45
Par/Crossed 1	22.5	90	90
Par/Crossed 2	45	90	90
Par/Crossed 3	67.5	90	90

Table 1: Angular descriptions of all configurations.

The N_2-H_2 interaction is defined by the center-of-mass intermolecular distance, R, and three angles; θ_1 and θ_2 are the in-plane angles of the molecules in relation to the z axis and ϕ_{12} is the relative torsion, or dihedral, angle between the molecules. The energy of the N_2-H_2 dimer, N_2, and H_2 were calculated separately for each configuration. For each of those sets, the distance of the interaction, R, was varied from 5 bohr to 12 bohr, in one-bohr increments. The H_2 bond length, *r*, was also varied from 1.25 to 1.55 bohr for additional calculations using the linear and T-shaped with H_2 horizontal. The additional R values 9.5, 10.5, and 11.5 bohr were used only for linear and T-shaped with H_2 horizontal configurations. Each set of parameters listed above was used to determine the dipole moments under the new conditions. The variation of the H_2 bond length mimics the vibrational component of the dimer. For each distance set the applied electric field was varied from -3E-3 to 3E-3 atomic units. Refer to Appendix for the

initial data. The least squares method for finding the linear regression was used to calculate the dipole moment from the BSSE-corrected interaction energies.

The above calculations were carried out using Dalton 2.0 (2005), a quantum chemical program used for the calculation of molecular properties including the wave function. The strengths of the program are mainly in the areas of magnetic and electric properties, and for studies of molecular potential energy surfaces, in this particular case the interaction-induced dipole moment. The program is based on solving the time-independent Schrödinger-equation:

$$\hat{H}\Psi = E\Psi \qquad (3)$$

From Eqn. 3, the wavefunction Ψ and energy E of an atom or molecule can be obtained. Using Dalton, a detailed description of chemical systems can be analyzed. It works primarily for small systems, such as the N_2-H_2 dimer, and can produce highly accurate calculations.[13]

BASIS SET SUPERPOSITION ERROR

The "basis set superposition error" (BSSE) is the discrepancy created by the overlapping of the atomic basis set functions as the molecules approach one another either by intermolecular or intramolecular interactions. As the atoms approach one another, they tend to borrow the basis functions from the opposing atom to create a larger basis set to improve the energy calculation. In this research, the interaction potential was determined by subtracting the N_2 and H_2 energy components from the dimer energy. This method is known as the "counterpoise method" developed by Boys and Bernardi[14], which removes the BSSE.[15]

QUANTUM CHEMICAL METHOD

The coupled cluster approach is used to add electron correlation to the wavefunction resulting in an increase in the accuracy of the calculations. Determining the molecular properties of many small molecules is "generally well-understood, and coupled cluster methods –particularly the CCSD(T) approach –in conjunction with large basis sets, have been found to give exceptionally accurate results relative to experiment for properties such as molecular geometries, harmonic vibrational frequencies, infrared intensities, and electric dipole moments".[16] Coupled cluster theory essentially uses the Hartree–Fock molecular orbital method and constructs multi-electron wavefunctions to account for electron correlation. Some of the most accurate calculations for small to medium sized molecules use this method. The classic example uses hydrogen molecules. Both the CCSD, coupled cluster single and double excitations, and CISD, configuration interaction single and double excitations, wavefunctions are exact (within the given one-electron basis set) for a single H_2 molecule since there are only two electrons to be correlated. However, errors are introduced in the CI energy in the case of two (or more) non-interacting H_2 units due to the lack of multiplicative separability of the wavefunction. The size consistent CCSD method produces the correct total energy, regardless of the number of non-interacting H_2 monomers in the system, since the total coupled cluster wavefunction may be written as a product of separated wavefunctions, each of which is exact for the given hydrogen molecule. In this study, the structure of the coupled cluster and configuration interaction wavefunctions for the system involve two initially separated components H_2 and N_2. If the molecular orbitals used to define the cluster functions are localized on each of the two molecules, a choice which will not affect the energy associated with either the reference determinant or the correlated wavefunction, the sum

of the energies computed for each fragment molecule separately is the same as that computed for the "super molecule" in which the fragments are included together in the calculation. This is called size consistency.[16]

LEAVE-ONE-OUT CROSS VALIDATION

In an attempt to obtain a good fit for the specified configurations, it is necessary to choose a functional form that is flexible enough to replicate the anisotropy of the system. From the previous work of Diep and Johnson,[17] the intermolecular potential is defined below by Eqn. 4. The most significant $\hat{G}_{l_1,l_2,l}$ contributors for the $(H_2)_2$ dimer are the first four-terms in the spherical harmonic expansion listed in Eqns. 5-8. The aim of the calculations presented here was to determine if these four terms would provide an accurate estimation of the N_2-H_2 interaction potential.

$$V(R,\Theta_1,\Theta_2,\Phi_{12}) = \sum_{l_1,l_2,l} V_{l_1,l_2,l}(R) G_{l_1,l_2,l}(\Theta_1,\Theta_2,\Phi_{12}) \qquad \textbf{(4)}$$

In Eqn. 4, the $V_{l1,l2,l}$ (R) are the functions of center-of-mass distance and the angular dependencies are accounted for by combinations of spherical harmonics.

$$G_{000}(\Theta_1,\Theta_2,\Phi_{12}) = 1 \qquad \textbf{(5)}$$

$$G_{202}(\Theta_1,\Theta_2,\Phi_{12}) = \frac{5}{2}(3\cos^2(\Theta_1) - 1) \qquad \textbf{(6)}$$

$$G_{022}(\Theta_1,\Theta_2,\Phi_{12}) = \frac{5}{2}(3\cos^2(\Theta_2) - 1) \qquad \textbf{(7)}$$

$$G_{224}(\Theta_1,\Theta_2,\Phi_{12}) = \frac{45}{4\sqrt{70}}[2(3\cos^2(\Theta_1) - 1)(3\cos^2(\Theta_2) - 1) - 16\sin(\Theta_1)\cos(\Theta_1)\sin(\Theta_2)\cos(\Theta_2)\cos(\Phi_{12}) + \sin^2(\Theta_1)\sin^2(\Theta_2)\cos(2\Phi_{12})] \qquad \textbf{(8)}$$

Consequently, the $G_{224}(\Theta_1,\Theta_2,\phi_{12})$ term of the expansion has the same angular dependence as the electrostatic quadrupole-quadrupole interaction defined below in Eqn. 9 .

$$E^{Q-Q} = \frac{3Q_1Q_2}{4R^5}[2(3\cos^2(\theta_1)-1)(3\cos^2(\theta_2)-1) - 16\sin(\theta_1)\cos(\theta_1) \sin(\theta_2)\cos(\theta_2)\cos(\phi_{12}) + \sin^2(\theta_1)\sin^2(\theta_2)\cos(2\phi_{12})] \quad \textbf{(9)}$$

After the Leave-one-out Cross Validation method described below was used to calculate the estimated values of the interaction energies at zero applied field, additional calculations were carried out for the parallel and crossed configurations. However, three angles of θ_1 for N_2 (22.5°, 45°, and 67.5°) were used to calculate the energies of the dimer, N_2, and H_2 at three different R values (5, 7, and 10 bohr). The varying angle represents three equal angles between the parallel and crossed orientations. Refer to Table 1 for angular descriptions of configurations.

Next, seven additional configurations (referred to below in Fig. 2 as configurations A through G) were used. The same R values from above and an electric field of zero were used; however, the angles of rotation remained fixed at 45°. Refer to Table 1 for angular descriptions of configurations.

The Leave-one-out Cross Validation method is a statistical method that can be used to calculate coefficients when the number of unknowns does not equal the number of equations. In this case, there are five configurations that must be fit with an equation that has four unknown coefficients. The Leave-one-out Cross Validation method eliminates one piece of data to create a situation with as many pieces of data as

coefficients. It is then possible to find the coefficients and use their values to make a prediction for the configuration that was left out. This is carried out five times, each time leaving out a different configuration. If the fitting equation is sufficient, it would be expected to have a very small error in all five predictions, and the coefficient values should be approximately the same in all five cases.

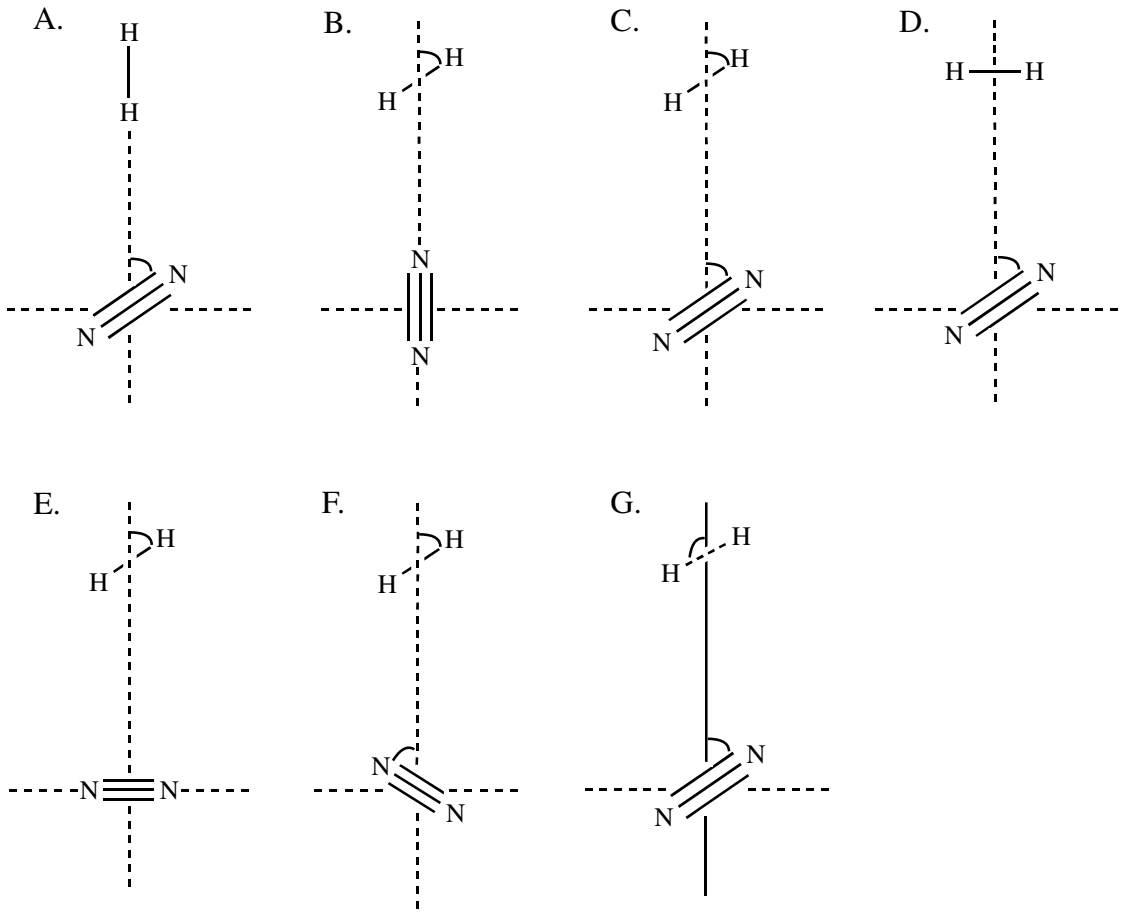

Figure 2: Diagram of the seven additional configurations, referred to as A through G. Refer to Table 1 for angular description.

RESULTS AND DISCUSSION

After Leave-one-out Cross Validation was performed, the estimated values of the interaction energies could be compared to the actual energies. Percent error analysis was used to determine the accuracy of using the Leave-one-out Cross Validation method

using the G functions G_{000}, G_{202}, G_{022}, and G_{224}. Tables 3 through 10 provide a comparison between the actual energies, calculated by Dalton, and estimated energies, calculated from the Leave-one-out Cross Validation. It is clear that there is a high percent difference between the values at every value of R.

It was anticipated that the coefficients (V_{000}, V_{022}, V_{202}, V_{224}) would be similar for the five different fits. However, there is some disparity among them. Refer to table 2 below for comparison. The T-shaped configurations have the same V_{000} coefficients and the parallel and crossed configurations are approximately close with an average 4% difference. However, the linear V_{000} coefficients vary significantly from the other four fits. Also, the estimated values for the interaction energies for each of the five fits are not in good agreement with the actual values from the calculations.

R (bohr)	Linear	T1	T2	Parallel	Crossed
5.0	9.01E-03	8.62E-03	8.62E-03	8.37E-03	8.30E-03
6.0	8.99E-04	9.70E-04	9.70E-04	9.45E-04	9.39E-04
7.0	-4.90E-05	-7.64E-05	-7.64E-05	-6.03E-05	-5.62E-05
8.0	-9.71E-05	-1.17E-04	-1.17E-04	-1.05E-04	-1.02E-04
9.0	-5.61E-05	-6.70E-05	-6.70E-05	-6.06E-05	-5.89E-05
10.0	-5.09E-05	-3.53E-05	-3.53E-05	-3.21E-05	-3.13E-05
11.0	-1.63E-05	-1.91E-05	-1.91E-05	-1.74E-05	-1.70E-05
12.0	-9.36E-06	-1.08E-05	-1.08E-05	-9.96E-06	-9.74E-06

Table 2: Comparison of the V_{000} coefficients for each of the five fits.

This was expected at low R values, around 5 to 7 bohr, but it was unexpected that the same situation persisted at large R values, around 10 to 12 bohr. In the close range, it is not uncommon that more terms are needed in the angular expansion of the potential energy function because the deformations of the molecular orbitals due to intermolecular

interactions can be reasonably substantial. However, the data suggests that additional terms are needed even at large R values. Also, the data presents some others trends that may be of interest, such as the T2 configuration consecutively has a relatively large fractional error. This may indicate that there is a way to improve the accuracy; however, it is difficult to determine without continuing with more calculations at lower and higher R values and with different configurations.

	Linear	**T-shaped 1**	**T-shaped 2**	**Parallel**	**Crossed**
Actual Energies:	0.020510277	0.018066659	0.004026069	0.002563588	0.002594378
Estimated Energies:	0.021680258	0.019340296	0.005299706	0.002713431	0.002460309
Error:	5.7%	7.04%	24.03%	5.52%	5.17%

Table 3: Error analysis of the estimated energies. Values for R = 5 Bohr.

	Linear	**T-shaped 1**	**T-shaped 2**	**Parallel**	**Crossed**
Actual Energies:	0.002496145	0.002582822	0.000336236	6.973E-06	6.4165E-05
Estimated Energies:	0.002282094	0.002710196	0.00046361	2.19585E-05	5.07569E-05
Error:	8.58%	4.93%	37.88%	214.91%	20.90%

Table 4: Error analysis of the estimated energies. Values for R = 6 Bohr.

	Linear	**T-shaped 1**	**T-shaped 2**	**Parallel**	**Crossed**
Actual Energies:	-0.000102646	0.000206791	-8.1963E-05	-0.000184926	-0.00015019
Estimated Energies:	-2.02E-05	0.000124377	-1.64E-04	-1.95E-04	-1.42E-04

Error:	80.32%	39.85%	100.10%	5.44%	5.45%

Table 5: Error analysis of the estimated energies. Values for R = 7 Bohr.

	Linear	T-shaped 1	T-shaped 2	Parallel	Crossed
Actual Energies:	-0.00025181	-4.9737E-05	-7.4731E-05	-0.000117716	-9.808E-05
Estimated Energies:	-1.93E-04	-1.08E-04	-1.33E-04	-1.25E-04	-9.19E-05
Error:	23.34%	117.14%	77.97%	6.19%	6.30%

Table 6: Error analysis of the estimated energies. Values for R = 8 Bohr.

	Linear	T-shaped 1	T-shaped 2	Parallel	Crossed
Actual Energies:	-0.00015257	-4.087E-05	-3.4542E-05	-6.4182E-05	-5.2759E-05
Estimated Energies:	-1.20E-04	-7.37E-05	-6.74E-05	-6.80E-05	-4.93E-05
Error:	21.3%	80.32%	95.12%	5.95%	6.56%

Table 7: Error analysis of the estimated energies. Values for R = 9 Bohr.

	Linear	T-shaped 1	T-shaped 2	Parallel	Crossed
Actual Energies:	-8.3617E-05	-2.0756E-05	-1.6247E-05	-0.000035417	-2.8477E-05
Estimated Energies:	-1.30E-04	-2.6854E-05	-3.23E-05	-3.73E-05	-2.68E-05
Error:	55.47%	29.37%	98.81%	5.32%	5.89%

Table 8: Error analysis of the estimated energies. Values for R = 10 Bohr.

	Linear	T-shaped 1	T-shaped 2	Parallel	Crossed
Actual Energies:	-4.7032E-05	-9.808E-06	-7.699E-06	-2.0461E-05	-1.6066E-05
Estimated Energies:	-3.88E-05	-1.80E-05	-1.59E-05	-2.14E-05	-1.52E-05

Error:	4.11%	83.52%	106.52%	4.59%	5.39%

Table 9: Error analysis of the estimated energies. Values for R = 11 Bohr.

	Linear	T-shaped 1	T-shaped 2	Parallel	Crossed
Actual Energies:	-2.7827E-05	-4.721E-06	-3.736E-06	-1.2404E-05	-9.517E-06
Estimated Energies:	-2.35E-05	-9.07E-06	-8.08E-06	-1.29E-05	-9.06E-06
Error:	15.55%	92.12%	116.27%	4.03%	4.80%

Table 10: Error analysis of the estimated energies. Values for R = 12 Bohr.

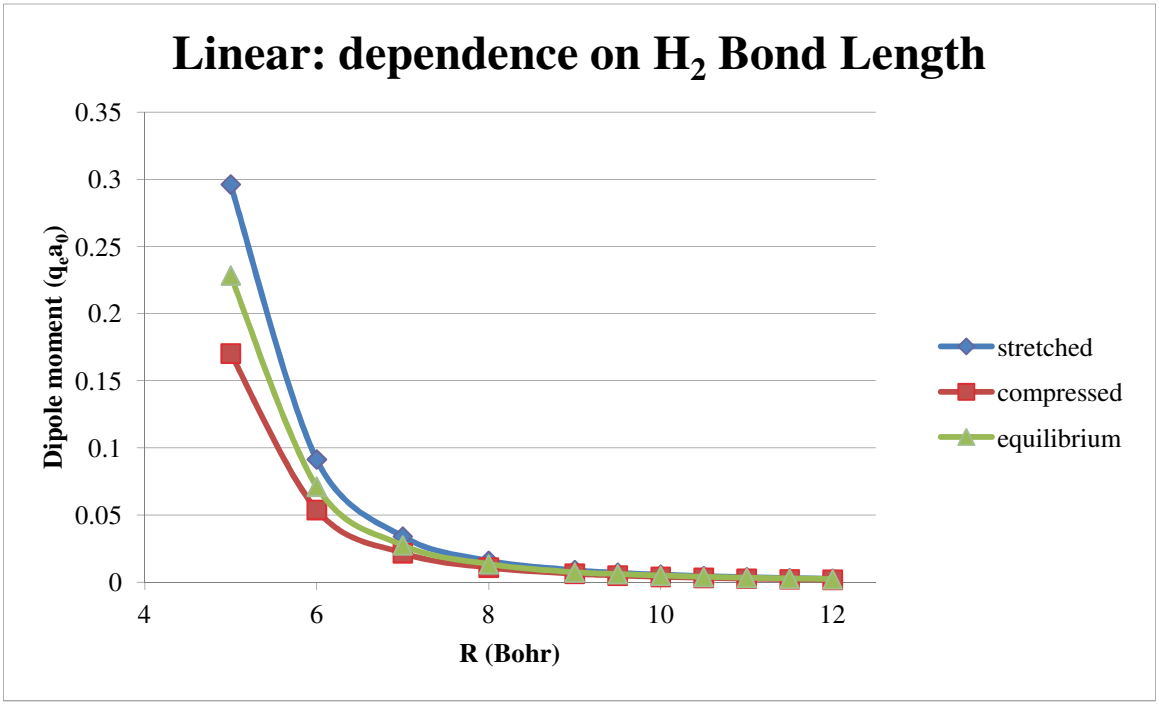

Figure 3: Comparison of the dipole moment magnitude for the stretched, compressed, and equilibrium H_2 bond length in the linear configuration.

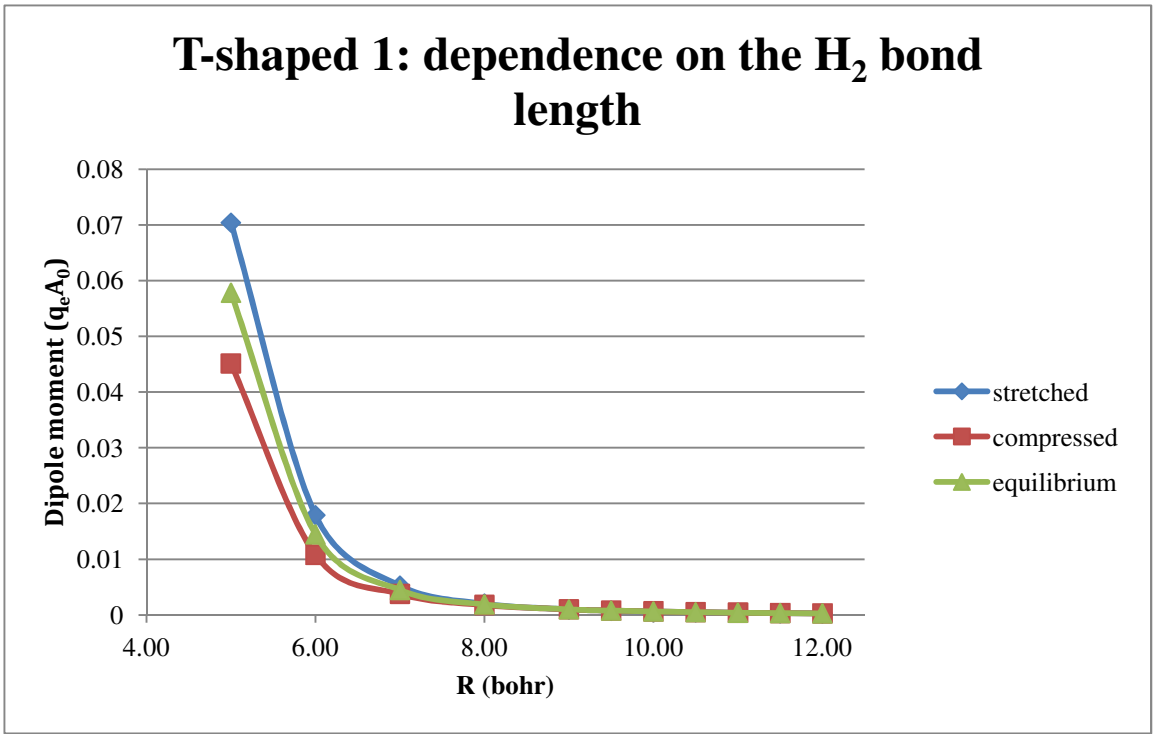

Figure 4: Comparison of the dipole moment magnitude for the stretched, compressed, and equilibrium H_2 bond length in the T-shaped 1 configuration.

From Figs. 3 and 4, it was observed that at large R values (9 to 12 Bohr), the dipole moment for each of the five initial configurations is minimal, as predicted. This is because as the interaction separation becomes larger, the molecules are moving away from each other and have less interaction. The dipole moment increases significantly as the R value is decreased, mimicking a collisional event. The dipole moment is larger for the stretched H_2 bond length than for the equilibrium and compressed bond lengths, with the compressed having the smallest dipole moment shift at low intermolecular separation. Varying the bond length mimics the vibrational motion of the H_2 molecule, resulting from the absorption of infrared radiation as in the case of atmospheric gases that absorb radiation from the sun.

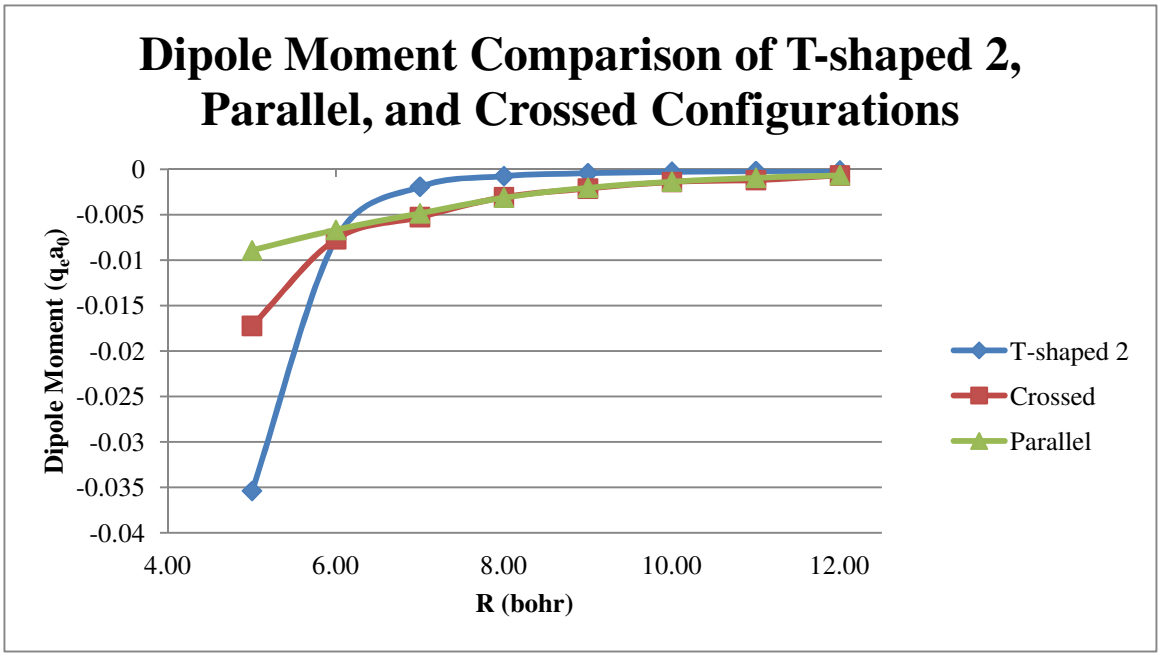

Figure 5: Comparison of the dipole moment magnitude for the T-Shaped 2, parallel, and crossed configurations at equilibrium bond length.

The data from Fig. 5 indicates that the magnitude of the dipole moment of the T-Shaped 2 (with N_2 horizontal) configuration at 0.04 q_eA_0 is the largest. However, the parallel configuration has a minimal dipole shift across the entire range of R values with the peak at 0.01 q_eA_0. These values are the absolute values of the collision-induced dipole moment. In comparison with equilibrium H_2 bond lengths from Figs. 3 and 4, the magnitude of the linear configuration dipole moment, 0.22 q_eA_0, is considerably larger than any of the other configurations.

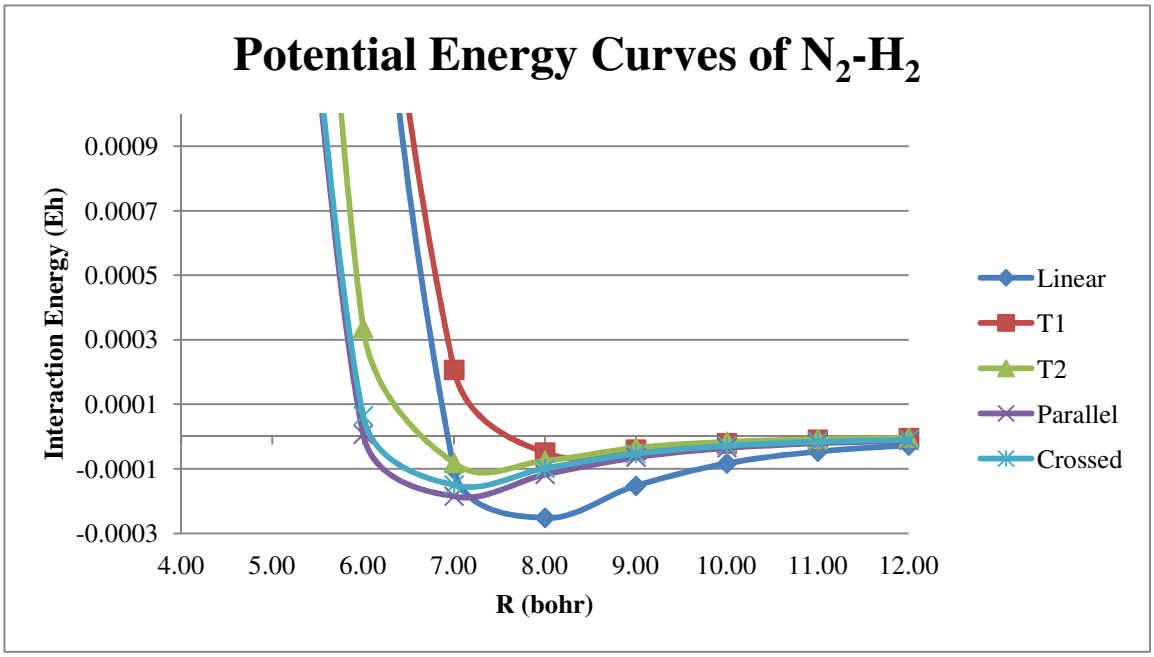

Figure 6: BSSE-corrected interaction energy comparison of the initial five configurations of N_2-H_2 at zero applied electric field.

From the potential energy curves of the initial five configurations, Fig. 6, it was determined that the minimum configuration is the linear configuration. The T-shaped 1 (with H_2 horizontal) is the most repulsive of the initial configurations. The potential curves of the other configurations lie between. The anisotropy of the potential energy surface is relatively small.

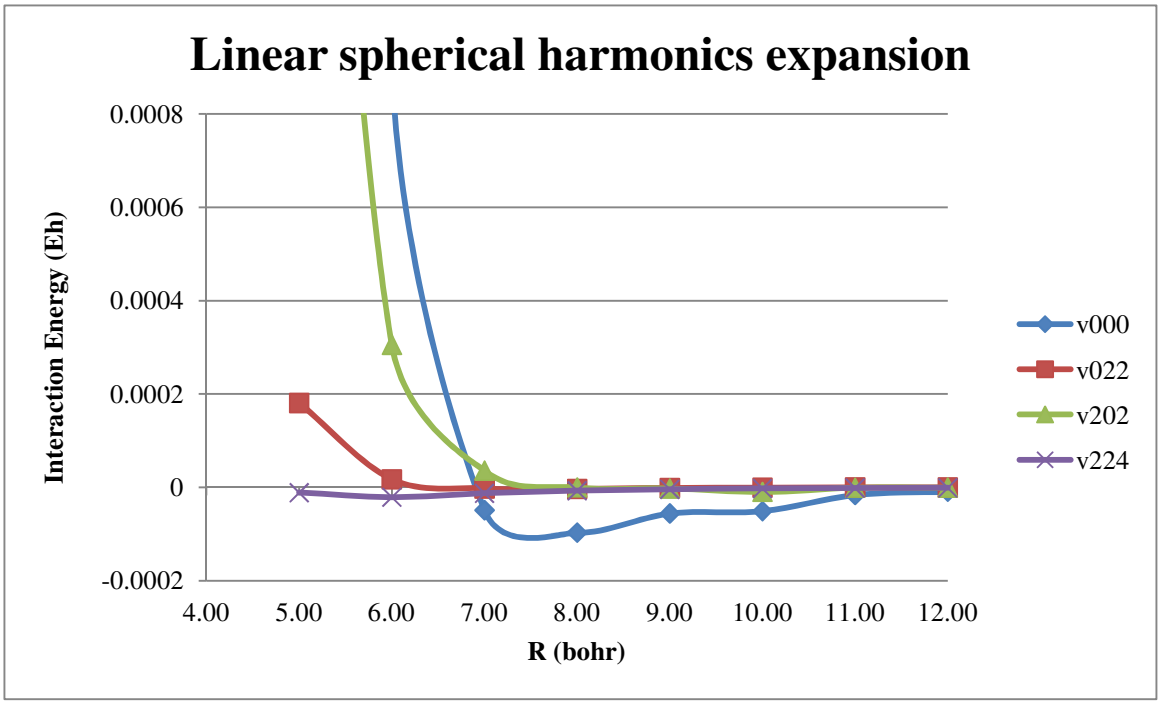

Figure 7: Values of the four-term spherical harmonics expansion.

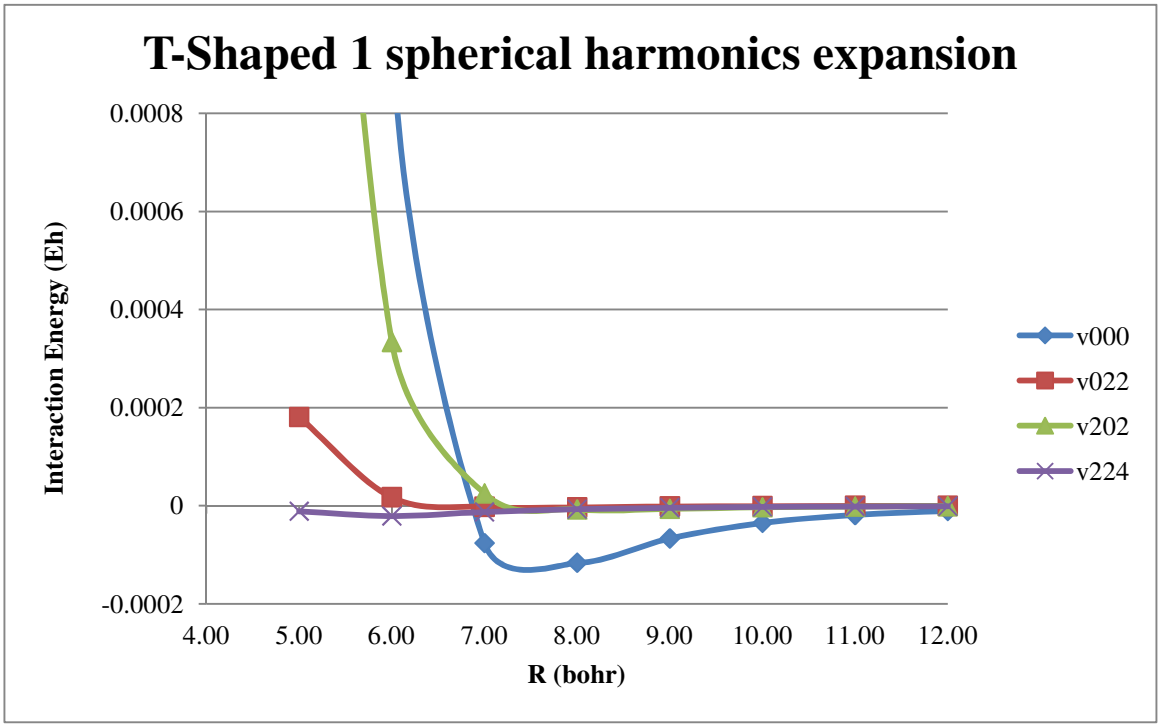

Figure 8: Values of the four-term spherical harmonics expansion.

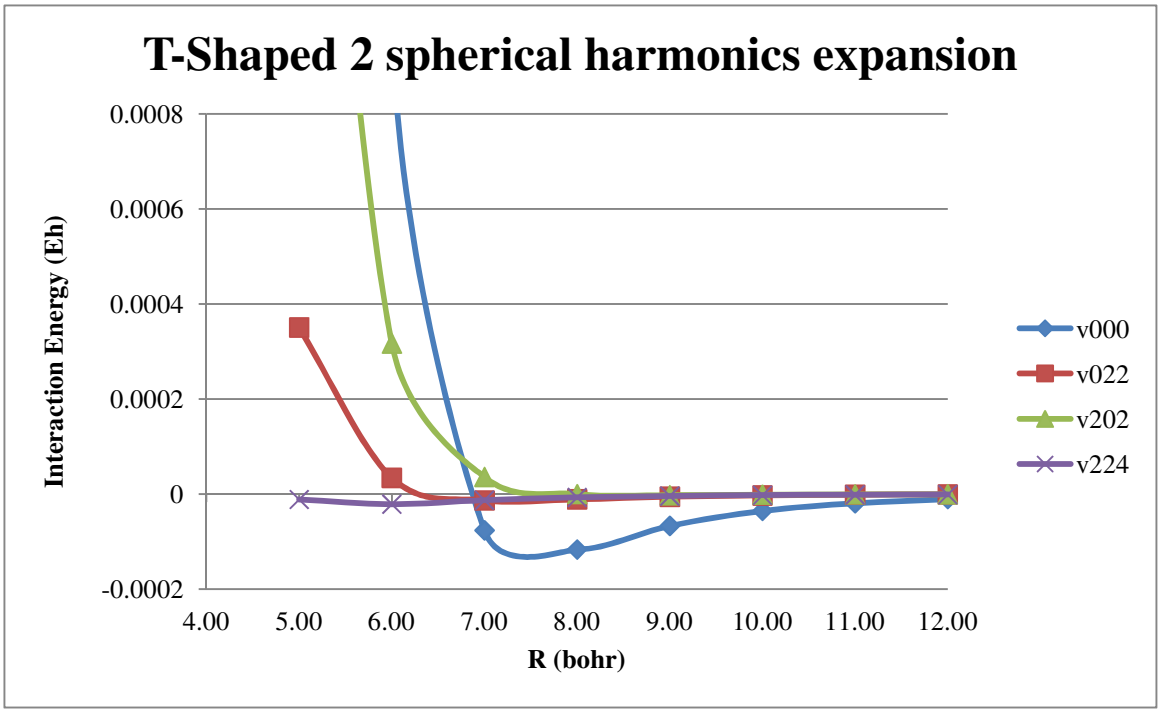

Figure 9: Values of the four-term spherical harmonics expansion.

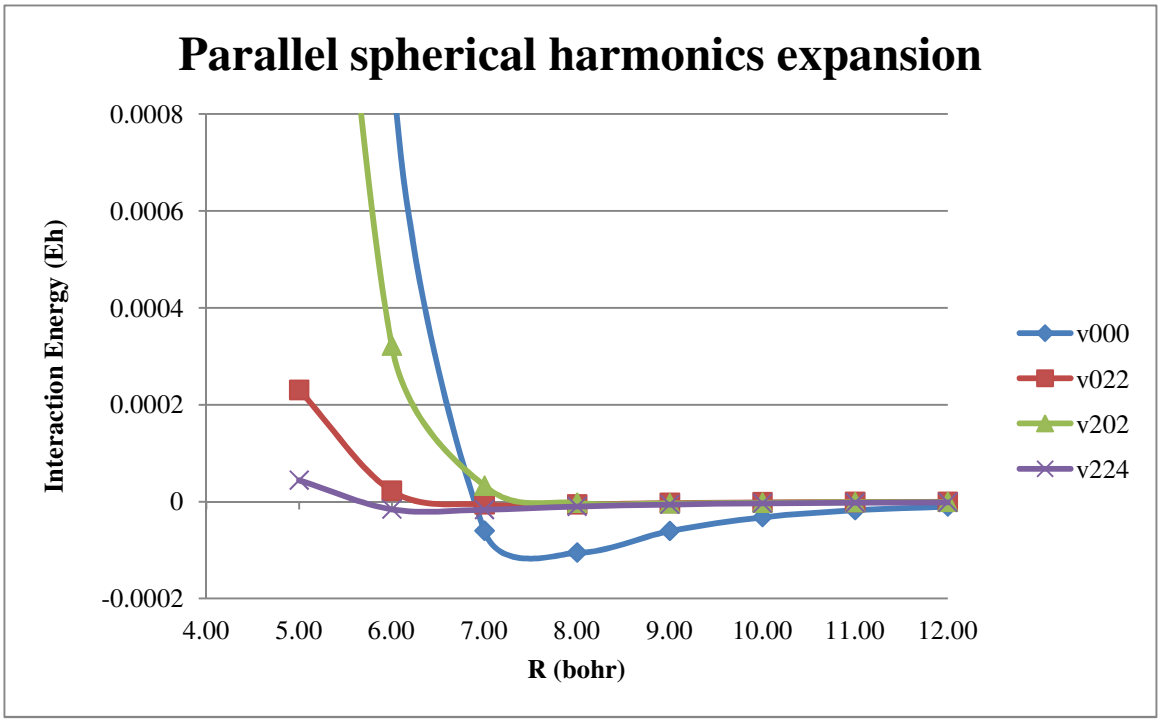

Figure 10: Values of the four-term spherical harmonics expansion.

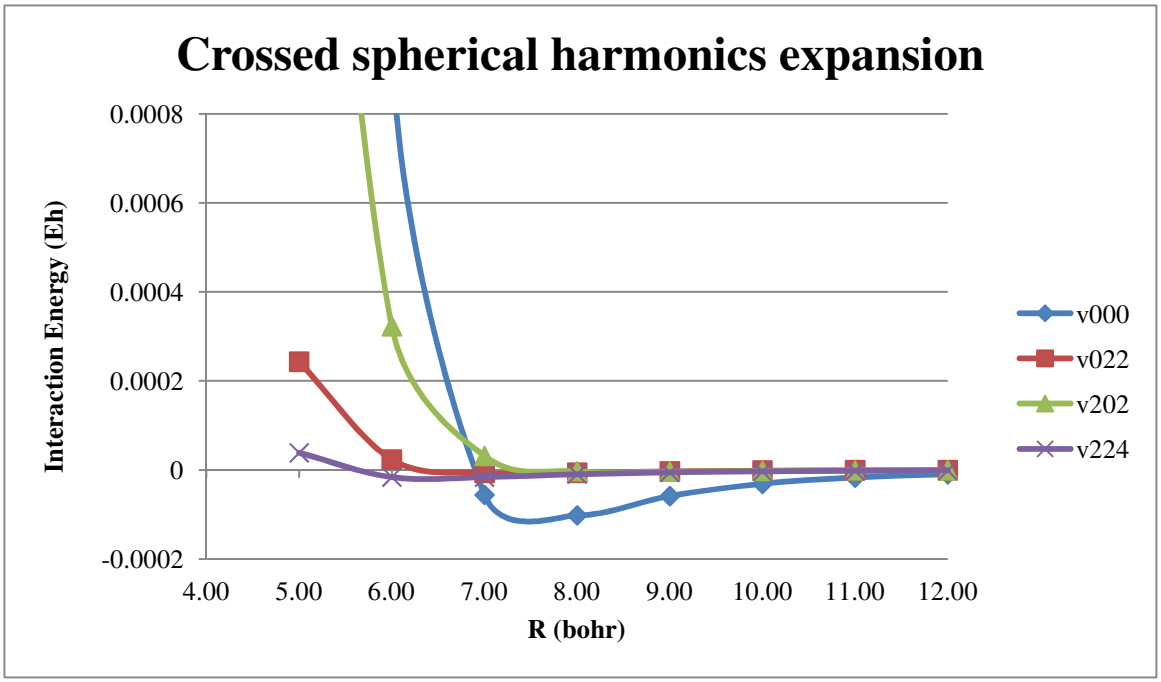

Figure 11: Values of the four-term spherical harmonics expansion.

From Figs. 7 through 11, it can be determined that the V_{000}, V_{022}, V_{202}, and V_{224} coefficients were different for each of the fits, which is inconsistent with what the results should have been from the Leave-one-out Cross Validation method.

CONCLUSION

From the Leave-one-out Cross Validation method, it was determined that the first four terms of the spherical harmonic expansion, G_{000}, G_{202}, G_{022}, and G_{224}, do not provide accurate estimated energy values for the N_2-H_2 interaction as they did for the H_2-H_2 interaction calculated by Diep and Johnson. This was determined by the high percent error, refer to Tables 3 through 10, between the actual energies and estimated energies. However, the next two terms in the expansion, G_{220} and G_{222} (Eqns. 10 and 11) may provide a more accurate estimation of the interaction energy. Further calculations need to be carried out to determine whether including those functions will provide more accurate

estimates of the interaction.

$$G_{220} = \frac{\sqrt{5}}{4}[(1-3\cos^2\theta_1)(1-3\cos^2\theta_2) + 3\cos 2\phi_{12}(1-\cos^2\theta_1\cos^2\theta_2) + 12\sin\theta_1\sin\theta_2\cos\theta_1\cos\theta_2\cos\phi_{12}] \quad \textbf{(10)}$$

$$G_{222} = -5\sqrt{\frac{5}{14}}[2-3\cos^2\theta_1 - 3\cos^2\theta_2 + 6\cos^2\theta_1\cos^2\theta_2 - 3\sin^2\theta_1\sin^2\theta_2\cos^2\phi_{12} + 3\sin\theta_1\sin\theta_2\cos\theta_1\cos\theta_2\cos\phi_{12}] \quad \textbf{(11)}$$

Also, the Leave-one-out Cross Validation method did not provide accurate V_{000}, V_{022}, V_{202}, and V_{224} coefficients. For each of the fits, the coefficients varied.

It can also be concluded from Figs. 3 through 5 at large R values, the dipole moment for each of the five initial configurations is minimal, as predicted. The dipole moment increases significantly as the R value is decreased, which is consistent with the theory that collisional interactions produced a measureable shift in the dipole moment of in the interaction of N_2 and H_2, nonpolar molecules. The dipole moment is also larger for the stretched H_2 bond length than for the equilibrium and compressed bond lengths, with the compressed having the smallest dipole moment shift at low intermolecular distance. Refer to Figs. 3 and 4 for a comparison of the linear configuration and T-shaped 1 (with H_2 horizontal) H_2 bond length dependence. This is because compressing the hydrogen bond would allow less space for the electrons to shift during dimer formation, creating less of a dipole moment shift. When the H_2 bond length is stretched, the electrons can shift more easily and the measured dipole moment is much larger.

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APPENDIX

The following tables are the initial data for each of the five configurations with H_2 bond length at 1.4011 bohr.

LINEAR						
R(Bohr)	Field	Dimer energy	N_2 energy	H_2 energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.545218466	-109.362272976	-1.202759002	0.019813512	
5.0	-0.002	-110.534931161	-109.362236282	-1.192743181	0.020048302	
5.0	-0.001	-110.524667551	-109.362214296	-1.182733807	0.020280552	
5.0	0.000	-110.514427589	-109.362207017	-1.172730849	0.020510277	
5.0	0.001	-110.504211228	-109.362214444	-1.162734306	0.020737522	
5.0	0.002	-110.494018426	-109.362236579	-1.152744179	0.020962332	
5.0	0.003	-110.483849144	-109.362273420	-1.142760508	0.021184784	0.001371272
6.0	-0.003	-110.568454576	-109.362002440	-1.208727657	0.002275521	
6.0	-0.002	-110.556326870	-109.361965804	-1.196711732	0.002350666	
6.0	-0.001	-110.544221890	-109.361943877	-1.184702222	0.002424209	
6.0	0.000	-110.532139640	-109.361936660	-1.172699125	0.002496145	
6.0	0.001	-110.520080020	-109.361944153	-1.160702441	0.002566574	
6.0	0.002	-110.508043092	-109.361966354	-1.148712171	0.002635433	
6.0	0.003	-110.496028813	-109.362003267	-1.136728317	0.002702771	0.000427250
7.0	-0.003	-110.576746358	-109.361866184	-1.214689995	-0.000190179	
7.0	-0.002	-110.562663390	-109.361829555	-1.200673982	-0.000159853	
7.0	-0.001	-110.548602696	-109.361807633	-1.186664383	-0.000130680	
7.0	0.000	-110.534564263	-109.361800421	-1.172661196	-0.000102646	
7.0	0.001	-110.520548084	-109.361807914	-1.158664422	-0.000075748	
7.0	0.002	-110.506554152	-109.361830128	-1.144674061	-0.000049963	
7.0	0.003	-110.492582461	-109.361867048	-1.130690130	-0.000025283	0.000164896
8.0	-0.003	-110.582750682	-109.361785076	-1.220672145	-0.000293461	
8.0	-0.002	-110.566682613	-109.361748384	-1.204656137	-0.000278092	
8.0	-0.001	-110.550636490	-109.361726404	-1.188646543	-0.000263543	
8.0	0.000	-110.534612306	-109.361717135	-1.172643361	-0.000251810	
8.0	0.001	-110.518610057	-109.361726517	-1.156646592	-0.000236948	
8.0	0.002	-110.502629740	-109.361748728	-1.140656235	-0.000224777	
8.0	0.003	-110.486671352	-109.361785591	-1.124672292	-0.000213469	0.000079992
9.0	-0.003	-110.588579883	-109.361733415	-1.226668488	-0.000177980	
9.0	-0.002	-110.570518009	-109.361696592	-1.208652485	-0.000168932	
9.0	-0.001	-110.552477838	-109.361674479	-1.190642896	-0.000160463	
9.0	0.000	-110.534459367	-109.361667077	-1.172639720	-0.000152570	
9.0	0.001	-110.516462601	-109.361674379	-1.154642956	-0.000145266	

9.0	0.002	-110.498487524	-109.361696400	-1.136652604	-0.000138520	
9.0	0.003	-110.480534144	-109.361733127	-1.118668667	-0.000132350	0.000045630
9.5	-0.003	-110.591513494	-109.361712677	-1.229667698	-0.000133119	
9.5	-0.002	-110.572453439	-109.361675805	-1.210651699	-0.000125935	
9.5	-0.001	-110.553414996	-109.361653642	-1.191642114	-0.000119240	
9.5	0.000	-110.534398163	-109.361646189	-1.172638941	-0.000113033	
9.5	0.001	-110.515402937	-109.361653444	-1.153642181	-0.000107312	
9.5	0.002	-110.496429319	-109.361675407	-1.134651834	-0.000102078	
9.5	0.003	-110.477477317	-109.361712080	-1.115667901	-0.000097336	0.000035783
10.0	-0.003	-110.594461667	-109.361694783	-1.232667120	-0.000099764	
10.0	-0.002	-110.574402971	-109.361657880	-1.212651125	-0.000093966	
10.0	-0.001	-110.554365814	-109.361635686	-1.192641543	-0.000088585	
10.0	0.000	-110.534350192	-109.361628200	-1.172638375	-0.000083617	
10.0	0.001	-110.514356104	-109.361635421	-1.152641619	-0.000079064	
10.0	0.002	-110.494383551	-109.361657351	-1.132651277	-0.000074923	
10.0	0.003	-110.474432533	-109.361693988	-1.112667349	-0.000071196	0.000028568
10.5	-0.003	-110.597422016	-109.361679760	-1.235666745	-0.000075511	
10.5	-0.002	-110.576364365	-109.361642845	-1.214650752	-0.000070768	
10.5	-0.001	-110.555328192	-109.361620638	-1.193641172	-0.000066382	
10.5	0.000	-110.534313493	-109.361613139	-1.172638006	-0.000062348	
10.5	0.001	-110.513320268	-109.361620346	-1.151641252	-0.000058670	
10.5	0.002	-110.492348517	-109.361642260	-1.130650911	-0.000055346	
10.5	0.003	-110.471398242	-109.361678882	-1.109666985	-0.000052375	0.000023136
11.0	-0.003	-110.600392627	-109.361668346	-1.238666393	-0.000057888	
11.0	-0.002	-110.578335803	-109.361631441	-1.216650399	-0.000053963	
11.0	-0.001	-110.556300407	-109.361609244	-1.194640818	-0.000050345	
11.0	0.000	-110.534286435	-109.361601754	-1.172637649	-0.000047032	
11.0	0.001	-110.512293888	-109.361608968	-1.150640894	-0.000044026	
11.0	0.002	-110.490322763	-109.361630889	-1.128650551	-0.000041323	
11.0	0.003	-110.468373065	-109.361667518	-1.106666623	-0.000038924	0.000018964
11.5	-0.003	-110.603371610	-109.361660647	-1.241665986	-0.000044977	
11.5	-0.002	-110.580315455	-109.361623770	-1.218649988	-0.000041697	
11.5	-0.001	-110.557280687	-109.361601601	-1.195640403	-0.000038683	
11.5	0.000	-110.534267300	-109.361594137	-1.172637230	-0.000035933	
11.5	0.001	-110.511275298	-109.361601376	-1.149640470	-0.000033452	
11.5	0.002	-110.488304675	-109.361623322	-1.126650124	-0.000031229	
11.5	0.003	-110.465355440	-109.361659974	-1.103666191	-0.000029275	0.000015702

12.0	-0.003	-110.606356946	-109.361655948	-1.244665567	-0.000035431	
12.0	-0.002	-110.582301335	-109.361619107	-1.220649566	-0.000032662	
12.0	-0.001	-110.558267077	-109.361596970	-1.196639977	-0.000030130	
12.0	0.000	-110.534254166	-109.361589539	-1.172636800	-0.000027827	
12.0	0.001	-110.510262603	-109.361596810	-1.148640034	-0.000025759	
12.0	0.002	-110.486292386	-109.361618785	-1.124649683	-0.000023918	
12.0	0.003	-110.462343521	-109.361655466	-1.100665744	-0.000022311	0.000013120

T-SHAPED WITH H_2 HORIZONTAL						
R(Bohr)	Field	Dimer energy	N_2 energy	H_2 energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.546831991	-109.362006424	-1.202714836	0.017889269	
5.0	-0.002	-110.536723654	-109.361969769	-1.192703464	0.017949579	
5.0	-0.001	-110.526636111	-109.361947825	-1.182696690	0.018008404	
5.0	0.000	-110.516568441	-109.361940588	-1.172694512	0.018066659	
5.0	0.001	-110.506520926	-109.361948060	-1.162696930	0.018124064	
5.0	0.002	-110.496493548	-109.361970240	-1.152703945	0.018180637	
5.0	0.003	-110.486486298	-109.362007130	-1.142715557	0.018236389	0.000347120
6.0	-0.003	-110.567995585	-109.361845973	-1.208685635	0.002536023	
6.0	-0.002	-110.555931173	-109.361809298	-1.196674258	0.002552383	
6.0	-0.001	-110.543886829	-109.361787334	-1.184667477	0.002567982	
6.0	0.000	-110.531862545	-109.361780077	-1.172665290	0.002582822	
6.0	0.001	-110.519858312	-109.361787529	-1.160667697	0.002596914	
6.0	0.002	-110.507874127	-109.361809688	-1.148674698	0.002610259	
6.0	0.003	-110.495909984	-109.361846557	-1.136686294	0.002622867	0.000086844
7.0	-0.003	-110.576260196	-109.361776296	-1.214674213	0.000190313	
7.0	-0.002	-110.562205943	-109.361739579	-1.200662842	0.000196478	
7.0	-0.001	-110.548171668	-109.361717572	-1.186656067	0.000201971	
7.0	0.000	-110.534157366	-109.361710272	-1.172653885	0.000206791	
7.0	0.001	-110.520163036	-109.361717680	-1.158656298	0.000210942	
7.0	0.002	-110.506188673	-109.361739795	-1.144663304	0.000214426	
7.0	0.003	-110.492234280	-109.361776618	-1.130674905	0.000217243	0.000026930
8.0	-0.003	-110.582441393	-109.361717977	-1.220665649	-0.000057767	
8.0	-0.002	-110.566389943	-109.361681119	-1.204654257	-0.000054567	
8.0	-0.001	-110.550358323	-109.361658970	-1.188647462	-0.000051891	
8.0	0.000	-110.534346530	-109.361651530	-1.172645263	-0.000049737	
8.0	0.001	-110.518354562	-109.361658797	-1.156647660	-0.000048105	
8.0	0.002	-110.502382420	-109.361680772	-1.140654652	-0.000046996	

8.0	0.003	-110.486430102	-109.361717456	-1.124666240	-0.000046406	0.000011361
9.0	-0.003	-110.588381368	-109.361675224	-1.226660486	-0.000045658	
9.0	-0.002	-110.570331046	-109.361638349	-1.208649035	-0.000043662	
9.0	-0.001	-110.552300417	-109.361616162	-1.190642185	-0.000042070	
9.0	0.000	-110.534289487	-109.361608682	-1.172639935	-0.000040870	
9.0	0.001	-110.516298239	-109.361615907	-1.154642285	-0.000040047	
9.0	0.002	-110.498326682	-109.361637839	-1.136649234	-0.000039609	
9.0	0.003	-110.480374816	-109.361674479	-1.118660784	-0.000039553	0.000006105
9.5	-0.003	-110.591356004	-109.361663880	-1.229658725	-0.000033399	
9.5	-0.002	-110.572306055	-109.361627011	-1.210647253	-0.000031791	
9.5	-0.001	-110.553275746	-109.361604848	-1.191640383	-0.000030515	
9.5	0.000	-110.534265072	-109.361597391	-1.172638115	-0.000029566	
9.5	0.001	-110.515274044	-109.361604638	-1.153640449	-0.000028957	
9.5	0.002	-110.496302640	-109.361626590	-1.134647386	-0.000028664	
9.5	0.003	-110.477350876	-109.361663249	-1.115658925	-0.000028702	0.000004697
10.0	-0.003	-110.594338635	-109.361657329	-1.232657546	-0.000023760	
10.0	-0.002	-110.574288984	-109.361620490	-1.212646058	-0.000022436	
10.0	-0.001	-110.554258927	-109.361598357	-1.192639175	-0.000021395	
10.0	0.000	-110.534248580	-109.361590928	-1.172636896	-0.000020756	
10.0	0.001	-110.514257581	-109.361598203	-1.152639220	-0.000020158	
10.0	0.002	-110.494286292	-109.361620182	-1.132646150	-0.000019960	
10.0	0.003	-110.474334605	-109.361656866	-1.112657684	-0.000020055	0.000003705
10.5	-0.003	-110.597327261	-109.361653623	-1.235656824	-0.000016814	
10.5	-0.002	-110.576277848	-109.361616811	-1.214645329	-0.000015708	
10.5	-0.001	-110.555247991	-109.361594704	-1.193638440	-0.000014847	
10.5	0.000	-110.534237684	-109.361587300	-1.172636156	-0.000014228	
10.5	0.001	-110.513246931	-109.361594598	-1.151638478	-0.000013855	
10.5	0.002	-110.492275728	-109.361616600	-1.130645407	-0.000013721	
10.5	0.003	-110.471324081	-109.361653307	-1.109656943	-0.000013831	0.000002983
11.0	-0.003	-110.600319638	-109.361651239	-1.238656428	-0.000011971	
11.0	-0.002	-110.578270418	-109.361614446	-1.216644933	-0.000011039	
11.0	-0.001	-110.556240722	-109.361592358	-1.194638044	-0.000010320	
11.0	0.000	-110.534230544	-109.361584973	-1.172635763	-0.000009808	
11.0	0.001	-110.512239887	-109.361592288	-1.150638089	-0.000009510	
11.0	0.002	-110.490268750	-109.361614307	-1.128645022	-0.000009421	
11.0	0.003	-110.468317137	-109.361651030	-1.106656563	-0.000009544	0.000002427

11.5	-0.003	-110.603314166	-109.361649336	-1.241656211	-0.000008619	
11.5	-0.002	-110.580265101	-109.361612557	-1.218644718	-0.000007826	
11.5	-0.001	-110.557235533	-109.361590481	-1.195637832	-0.000007220	
11.5	0.000	-110.534225455	-109.361583107	-1.172635555	-0.000006793	
11.5	0.001	-110.511234873	-109.361590434	-1.149637885	-0.000006554	
11.5	0.002	-110.488263782	-109.361612463	-1.126644823	-0.000006496	
11.5	0.003	-110.465312189	-109.361649197	-1.103656387	-0.000006605	0.000002014
12.0	-0.003	-110.606309955	-109.361647623	-1.244656054	-0.000006278	
12.0	-0.002	-110.582261012	-109.361610852	-1.220644563	-0.000005597	
12.0	-0.001	-110.558231543	-109.361588750	-1.196637680	-0.000005113	
12.0	0.000	-110.534221543	-109.361581417	-1.172635405	-0.000004721	
12.0	0.001	-110.510231014	-109.361588750	-1.148637737	-0.000004527	
12.0	0.002	-110.486259955	-109.361610785	-1.124644678	-0.000004492	
12.0	0.003	-110.462308371	-109.361647524	-1.100656229	-0.000004618	0.000001660

T-SHAPED WITH N_2 HORIZONTAL						
R(bohr)	Field	Dimer energy	N_2 energy	H_2 energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.740719305	-109.572132950	-1.172712891	0.004126536	
5.0	-0.002	-110.670710238	-109.502107724	-1.172696799	0.004094285	
5.0	-0.001	-110.600718913	-109.432092595	-1.172687119	0.004060801	
5.0	0.000	-110.530745343	-109.362087560	-1.172683852	0.004026069	
5.0	0.001	-110.460789542	-109.292092620	-1.172686997	0.003990075	
5.0	0.002	-110.390851526	-109.222107778	-1.172696553	0.003952805	
5.0	0.003	-110.320931313	-109.151213303	-1.172712522	0.002994512	-0.001132024
6.0	-0.003	-110.786241316	-109.613914063	-1.172681993	0.000354740	
6.0	-0.002	-110.702205456	-109.529889053	-1.172665954	0.000349551	
6.0	-0.001	-110.618187081	-109.445874137	-1.172656328	0.000343384	
6.0	0.000	-110.534186195	-109.361869317	-1.172653114	0.000336236	
6.0	0.001	-110.450202802	-109.277874591	-1.172656313	0.000328102	
6.0	0.002	-110.366236909	-109.193889962	-1.172665923	0.000318976	
6.0	0.003	-110.282288525	-109.109915431	-1.172681946	0.000308852	-0.000045888
7.0	-0.003	-110.828522715	-109.655773169	-1.172670109	-0.000079437	
7.0	-0.002	-110.730481914	-109.557748306	-1.172654051	-0.000079557	
7.0	-0.001	-110.632458347	-109.459733541	-1.172644407	-0.000080399	
7.0	0.000	-110.534452015	-109.361728876	-1.172641176	-0.000081963	
7.0	0.001	-110.436462918	-109.263734309	-1.172644357	-0.000084252	
7.0	0.002	-110.338491058	-109.165749842	-1.172653951	-0.000087265	
7.0	0.003	-110.240536440	-109.067775477	-1.172669958	-0.000091005	-0.000011568

8.0	-0.003	-110.870434485	-109.697697824	-1.172668242	-0.000068419	
8.0	-0.002	-110.758393015	-109.585672940	-1.172652179	-0.000067896	
8.0	-0.001	-110.646368576	-109.473658161	-1.172642531	-0.000067884	
8.0	0.000	-110.534361167	-109.361653486	-1.172632950	-0.000074731	
8.0	0.001	-110.422370787	-109.249658960	-1.172642472	-0.000069355	
8.0	0.002	-110.310397437	-109.137674452	-1.172652061	-0.000070924	
8.0	0.003	-110.198441120	-109.025700095	-1.172668064	-0.000072961	-0.000004542
9.0	-0.003	-110.912364782	-109.739662947	-1.172666936	-0.000034899	
9.0	-0.002	-110.786323312	-109.613638021	-1.172650875	-0.000034416	
9.0	-0.001	-110.660298726	-109.487623201	-1.172641228	-0.000034297	
9.0	0.000	-110.534291022	-109.361618486	-1.172637994	-0.000034542	
9.0	0.001	-110.408300199	-109.235623876	-1.172641172	-0.000035151	
9.0	0.002	-110.282326256	-109.109639372	-1.172650763	-0.000036121	
9.0	0.003	-110.156369198	-108.983664976	-1.172666766	-0.000037456	-0.000002557
10.0	-0.003	-110.954328403	-109.781646161	-1.172665649	-0.000016593	
10.0	-0.002	-110.814287015	-109.641621208	-1.172649595	-0.000016212	
10.0	-0.001	-110.674262409	-109.501606357	-1.172639954	-0.000016098	
10.0	0.000	-110.534254581	-109.361601609	-1.172636725	-0.000016247	
10.0	0.001	-110.394263531	-109.221606962	-1.172639907	-0.000016662	
10.0	0.002	-110.254289258	-109.081622419	-1.172649502	-0.000017337	
10.0	0.003	-110.114331765	-108.941647979	-1.172665509	-0.000018277	-0.000001684
11.0	-0.003	-110.996310711	-109.823638029	-1.172664681	-0.000008001	
11.0	-0.002	-110.842269342	-109.669613001	-1.172648638	-0.000007703	
11.0	-0.001	-110.688244681	-109.515598071	-1.172639008	-0.000007602	
11.0	0.000	-110.534236727	-109.361593240	-1.172635788	-0.000007699	
11.0	0.001	-110.380245478	-109.207598506	-1.172638980	-0.000007992	
11.0	0.002	-110.226270934	-109.053613870	-1.172648584	-0.000008480	
11.0	0.003	-110.072313097	-108.899639331	-1.172664599	-0.000009167	-0.000001166
12.0	-0.003	-111.038298263	-109.865630342	-1.172663929	-0.000003992	
12.0	-0.002	-110.870256868	-109.697605215	-1.172647897	-0.000003756	
12.0	-0.001	-110.702232132	-109.529590184	-1.172638277	-0.000003671	
12.0	0.000	-110.534224053	-109.361585249	-1.172635068	-0.000003736	
12.0	0.001	-110.366232630	-109.193590409	-1.172638268	-0.000003953	
12.0	0.002	-110.198257863	-109.025605664	-1.172647879	-0.000004320	
12.0	0.003	-110.030299754	-108.857631015	-1.172663901	-0.000004838	-0.000000846

PARALLEL						
R(bohr)	Field	Dimer energy	N_2 energy	H_2 energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.561994101	-109.361884147	-1.202679613	0.002569659	
5.0	-0.002	-110.551958608	-109.361856060	-1.192668247	0.002565699	
5.0	-0.001	-110.541938418	-109.361843162	-1.182661475	0.002566219	
5.0	0.000	-110.531933522	-109.361837815	-1.172659295	0.002563588	
5.0	0.001	-110.521943916	-109.361842563	-1.162661706	0.002560353	
5.0	0.002	-110.511969595	-109.361857406	-1.152668710	0.002556521	
5.0	0.003	-110.502010554	-109.361882344	-1.142680306	0.002552096	-0.000017563
6.0	-0.003	-110.570406473	-109.361760323	-1.208670510	0.000024360	
6.0	-0.002	-110.558374712	-109.361734711	-1.196659150	0.000019149	
6.0	-0.001	-110.546358234	-109.361719203	-1.184652384	0.000013353	
6.0	0.000	-110.534357036	-109.361713797	-1.172650212	0.000006973	
6.0	0.001	-110.522371116	-109.361718493	-1.160652634	0.000000011	
6.0	0.002	-110.510400474	-109.361733290	-1.148659648	-0.000007536	
6.0	0.003	-110.498445109	-109.361758189	-1.136671256	-0.000015664	-0.000040024
7.0	-0.003	-110.576415369	-109.361679076	-1.214663821	-0.000072472	
7.0	-0.002	-110.562482071	-109.361653470	-1.200652443	-0.000176158	
7.0	-0.001	-110.548463946	-109.361637974	-1.186645662	-0.000180310	
7.0	0.000	-110.534460990	-109.361632586	-1.172643478	-0.000184926	
7.0	0.001	-110.520473203	-109.361637305	-1.158645890	-0.000190008	
7.0	0.002	-110.506500586	-109.361652132	-1.144652899	-0.000195555	
7.0	0.003	-110.492543140	-109.361677066	-1.130664504	-0.000201570	-0.000129098
8.0	-0.003	-110.582421010	-109.361651742	-1.220659408	-0.000109860	
8.0	-0.002	-110.566386267	-109.361626172	-1.204647958	-0.000112137	
8.0	-0.001	-110.550366573	-109.361610707	-1.188641110	-0.000114756	
8.0	0.000	-110.534361926	-109.361605346	-1.172638864	-0.000117716	
8.0	0.001	-110.518372326	-109.361610090	-1.156641220	-0.000121016	
8.0	0.002	-110.502397775	-109.361624938	-1.140648177	-0.000124660	
8.0	0.003	-110.486438274	-109.361649892	-1.124659736	-0.000128646	-0.000018786
9.0	-0.003	-110.588356730	-109.361640461	-1.226657071	-0.000059198	
9.0	-0.002	-110.570321201	-109.361650020	-1.208645586	-0.000025595	
9.0	-0.001	-110.552300625	-109.361599644	-1.190638707	-0.000062274	
9.0	0.000	-110.534295000	-109.361594384	-1.172636434	-0.000064182	
9.0	0.001	-110.516304326	-109.361599222	-1.154638766	-0.000066338	

9.0	0.002	-110.498328605	-109.361614160	-1.136645705	-0.000068740	
9.0	0.003	-110.480367839	-109.361639197	-1.118657251	-0.000071391	-0.000012193
10.0	-0.003	-110.594319909	-109.361631590	-1.232656159	-0.000032160	
10.0	-0.002	-110.574283971	-109.361606239	-1.212644668	-0.000033064	
10.0	-0.001	-110.554262920	-109.361590985	-1.192637785	-0.000034150	
10.0	0.000	-110.534256753	-109.361585826	-1.172635510	-0.000035417	
10.0	0.001	-110.514265472	-109.361590763	-1.152637843	-0.000036866	
10.0	0.002	-110.494289077	-109.361605796	-1.132644783	-0.000038498	
10.0	0.003	-110.474327571	-109.361630927	-1.112656333	-0.000040311	-0.000008151
11.0	-0.003	-110.600300006	-109.361625976	-1.238655767	-0.000018263	
11.0	-0.002	-110.578263815	-109.361600682	-1.216644275	-0.000018858	
11.0	-0.001	-110.556242466	-109.361585483	-1.194637392	-0.000019591	
11.0	0.000	-110.534235955	-109.361580379	-1.172635115	-0.000020461	
11.0	0.001	-110.512244285	-109.361585371	-1.150637447	-0.000021467	
11.0	0.002	-110.490267455	-109.361500457	-1.128644388	-0.000122610	
11.0	0.003	-110.468305469	-109.361635641	-1.106655938	-0.000013890	0.000004373
12.0	-0.003	-110.606289342	-109.361622977	-1.244655486	-0.000010879	
12.0	-0.002	-110.582252981	-109.361597710	-1.220643990	-0.000011281	
12.0	-0.001	-110.558231428	-109.361582536	-1.196637102	-0.000011790	
12.0	0.000	-110.534224683	-109.361577458	-1.172634821	-0.000012404	
12.0	0.001	-110.510232745	-109.361582474	-1.148637148	-0.000013123	
12.0	0.002	-110.486255616	-109.361597586	-1.124644082	-0.000013948	
12.0	0.003	-110.462293297	-109.361622793	-1.100655625	-0.000014879	-0.000004000

CROSSED						
R(bohr)	Field	Dimer energy	N_2 energy	H_2 energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.561966373	-109.361893503	-1.202681767	0.002608897	
5.0	-0.002	-110.551933637	-109.361867888	-1.192670407	0.002604658	
5.0	-0.001	-110.541916194	-109.361852371	-1.182663400	0.002599577	
5.0	0.000	-110.531914038	-109.361846952	-1.172661464	0.002594378	
5.0	0.001	-110.521927162	-109.361851630	-1.162663879	0.002588347	
5.0	0.002	-110.511955562	-109.361866403	-1.152670885	0.002581726	
5.0	0.003	-110.501999235	-109.361891272	-1.142682483	0.002574520	-0.000034377
6.0	-0.003	-110.570349642	-109.361763052	-1.208671246	0.000084656	
6.0	-0.002	-110.558318824	-109.361737348	-1.196659882	0.000078406	
6.0	-0.001	-110.546303287	-109.361721750	-1.184653113	0.000071576	
6.0	0.000	-110.534303028	-109.361716257	-1.172650936	0.000064165	
6.0	0.001	-110.522318044	-109.361720867	-1.160653353	0.000056176	

6.0	0.002	-110.510348336	-109.361735580	-1.148660362	0.000047606	
6.0	0.003	-110.498393902	-109.361760396	-1.136671965	0.000038459	-0.000046197
7.0	-0.003	-110.576481996	-109.361681256	-1.214664294	-0.000136446	
7.0	-0.002	-110.562449056	-109.361655582	-1.200652911	-0.000140563	
7.0	-0.001	-110.548431290	-109.361640020	-1.186646125	-0.000145145	
7.0	0.000	-110.534428697	-109.361634570	-1.172643937	-0.000150190	
7.0	0.001	-110.520441275	-109.361639232	-1.158646344	-0.000155699	
7.0	0.002	-110.506469024	-109.361654005	-1.144653348	-0.000161671	
7.0	0.003	-110.492511946	-109.361678890	-1.130664949	-0.000168107	-0.000031661
8.0	-0.003	-110.582403195	-109.361653884	-1.220659680	-0.000089631	
8.0	-0.002	-110.566368568	-109.361628229	-1.204648232	-0.000092107	
8.0	-0.001	-110.550348995	-109.361612686	-1.188641386	-0.000094923	
8.0	0.000	-110.534344472	-109.361607251	-1.172639141	-0.000098080	
8.0	0.001	-110.518355001	-109.361611925	-1.156641498	-0.000101578	
8.0	0.002	-110.502380581	-109.361626708	-1.140648456	-0.000105417	
8.0	0.003	-110.486421214	-109.361653884	-1.124660017	-0.000107313	-0.000017682
9.0	-0.003	-110.588346081	-109.361641446	-1.226657159	-0.000047476	
9.0	-0.002	-110.570310586	-109.361659190	-1.208645677	-0.000005719	
9.0	-0.001	-110.552290046	-109.361600494	-1.190638800	-0.000050752	
9.0	0.000	-110.534284460	-109.361595172	-1.172636529	-0.000052759	
9.0	0.001	-110.516293828	-109.361599951	-1.154638863	-0.000055014	
9.0	0.002	-110.498318152	-109.361614833	-1.136645803	-0.000057516	
9.0	0.003	-110.480357433	-109.361639818	-1.118657350	-0.000060265	-0.000012789
10.0	-0.003	-110.594313022	-109.361631816	-1.232656149	-0.000025057	
10.0	-0.002	-110.574277101	-109.361606426	-1.212644660	-0.000026015	
10.0	-0.001	-110.554256069	-109.361591135	-1.192637778	-0.000027156	
10.0	0.000	-110.534249922	-109.361585942	-1.172635503	-0.000028477	
10.0	0.001	-110.514258662	-109.361590846	-1.152637837	-0.000029979	
10.0	0.002	-110.494282291	-109.361605848	-1.132644778	-0.000031665	
10.0	0.003	-110.474320809	-109.361630949	-1.112656328	-0.000033532	-0.000008475
11.0	-0.003	-110.600295499	-109.361625990	-1.238655734	-0.000013775	
11.0	-0.002	-110.578259322	-109.361600678	-1.216644243	-0.000014401	
11.0	-0.001	-110.556237987	-109.361585463	-1.194637358	-0.000015166	
11.0	0.000	-110.534231492	-109.361580343	-1.172635083	-0.000016066	
11.0	0.001	-110.512239838	-109.361585319	-1.150637416	-0.000017103	
11.0	0.002	-110.490266303	-109.361600392	-1.128644357	-0.000021554	
11.0	0.003	-110.468301057	-109.361625562	-1.106655907	-0.000019588	-0.000005813

12.0	-0.003	-110.606286360	-109.361622967	-1.244655458	-0.000007935	
12.0	-0.002	-110.582250010	-109.361597689	-1.220643962	-0.000008359	
12.0	-0.001	-110.558228468	-109.361582509	-1.196637075	-0.000008884	
12.0	0.000	-110.534221735	-109.361577424	-1.172634794	-0.000009517	
12.0	0.001	-110.510229810	-109.361582433	-1.148637121	-0.000010256	
12.0	0.002	-110.486252693	-109.361597539	-1.124644055	-0.000011099	
12.0	0.003	-110.462290387	-109.361622741	-1.100655598	-0.000012048	-0.000004113

The following tables are the initial data for each of the five configurations with H_2 bond length at 1.55 bohr.

LINEAR						
R(bohr)	Field	Dimer Energy	N_2 Energy	H_2 Energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.540463179	-109.362288680	-1.199425336	0.021250837	
5.0	-0.002	-110.530104034	-109.362251981	-1.189407062	0.021555009	
5.0	-0.001	-110.519770284	-109.362229991	-1.179396283	0.021855990	
5.0	0.000	-110.509461862	-109.362222707	-1.169392902	0.022153747	
5.0	0.001	-110.499178707	-109.362230130	-1.159396965	0.022448388	
5.0	0.002	-110.488920760	-109.362252259	-1.149408474	0.022739973	
5.0	0.003	-110.478687968	-109.362289096	-1.139427430	0.023028558	0.001777721
6.0	-0.003	-110.564836062	-109.362011395	-1.205391058	0.002566391	
6.0	-0.002	-110.552684877	-109.361974757	-1.193372656	0.002662536	
6.0	-0.001	-110.540557775	-109.361952829	-1.181361698	0.002756752	
6.0	0.000	-110.528457280	-109.361945611	-1.169358182	0.002846513	
6.0	0.001	-110.516375705	-109.361953102	-1.157362109	0.002939506	
6.0	0.002	-110.504320681	-109.361975303	-1.145373480	0.003028102	
6.0	0.003	-110.492289631	-109.362012214	-1.133392248	0.003114831	0.000548440
7.0	-0.003	-110.573416652	-109.361870854	-1.211351652	-0.000194146	
7.0	-0.002	-110.559324035	-109.361834215	-1.197333106	-0.000156714	
7.0	-0.001	-110.545254921	-109.361812287	-1.183322003	-0.000120631	
7.0	0.000	-110.531209294	-109.361805069	-1.169318342	-0.000085883	
7.0	0.001	-110.517187139	-109.361812557	-1.155322122	-0.000052460	
7.0	0.002	-110.503188446	-109.361834766	-1.141333344	-0.000020336	
7.0	0.003	-110.489213209	-109.361871680	-1.127352009	0.000010480	0.000204626
8.0	-0.003	-110.579449587	-109.361786885	-1.217333903	-0.000328799	
8.0	-0.002	-110.563375953	-109.361750196	-1.201315335	-0.000310422	
8.0	-0.001	-110.547325427	-109.361728218	-1.185304209	-0.000293000	
8.0	0.000	-110.531297998	-109.361720951	-1.169300524	-0.000276523	
8.0	0.001	-110.515293666	-109.361728389	-1.153304281	-0.000260996	
8.0	0.002	-110.499312428	-109.361750548	-1.137315480	-0.000246400	
8.0	0.003	-110.483354277	-109.361787413	-1.121334122	-0.000232742	0.000096057

9.0	-0.003	-110.585265407	-109.361732889	-1.223330020	-0.000202498	
9.0	-0.002	-110.567199365	-109.361696066	-1.205311453	-0.000191846	
9.0	-0.001	-110.549156153	-109.361673955	-1.187300330	-0.000181868	
9.0	0.000	-110.531135761	-109.361666553	-1.169296649	-0.000172559	
9.0	0.001	-110.513138191	-109.361673855	-1.151300409	-0.000163927	
9.0	0.002	-110.495163441	-109.361695878	-1.133311612	-0.000155951	
9.0	0.003	-110.477211511	-109.361732605	-1.115330258	-0.000148648	0.000053850
9.5	-0.003	-110.588193029	-109.361711688	-1.226329335	-0.000152006	
9.5	-0.002	-110.569129164	-109.361674815	-1.207310771	-0.000143578	
9.5	-0.001	-110.550088023	-109.361652652	-1.188299650	-0.000135721	
9.5	0.000	-110.531069598	-109.361645198	-1.169295971	-0.000128429	
9.5	0.001	-110.512073890	-109.361652452	-1.150299734	-0.000121704	
9.5	0.002	-110.493100899	-109.361674414	-1.131310939	-0.000115546	
9.5	0.003	-110.474150624	-109.361711086	-1.112329588	-0.000109950	0.000042056
10.0	-0.003	-110.591137380	-109.361694315	-1.229328897	-0.000114168	
10.0	-0.002	-110.571075129	-109.361657413	-1.209310335	-0.000107381	
10.0	-0.001	-110.551035516	-109.361635220	-1.189299217	-0.000101079	
10.0	0.000	-110.531018532	-109.361627735	-1.169295540	-0.000095257	
10.0	0.001	-110.511024183	-109.361634958	-1.149299305	-0.000089920	
10.0	0.002	-110.491052460	-109.361656888	-1.129310513	-0.000085059	
10.0	0.003	-110.471103373	-109.361693527	-1.109329165	-0.000080681	0.000033487
10.5	-0.003	-110.594095118	-109.361679954	-1.232328629	-0.000086535	
10.5	-0.002	-110.573034098	-109.361643041	-1.211310068	-0.000080989	
10.5	-0.001	-110.551995645	-109.361620836	-1.190298950	-0.000075859	
10.5	0.000	-110.530979755	-109.361613339	-1.169295274	-0.000071142	
10.5	0.001	-110.509986421	-109.361620548	-1.148299040	-0.000066833	
10.5	0.002	-110.489015648	-109.361642464	-1.127310247	-0.000062937	
10.5	0.003	-110.468067441	-109.361679088	-1.106328899	-0.000059454	0.000027081
11.0	-0.003	-110.597063630	-109.361668850	-1.235328369	-0.000066411	
11.0	-0.002	-110.575003575	-109.361631945	-1.213309805	-0.000061825	
11.0	-0.001	-110.552966030	-109.361609749	-1.191298685	-0.000057596	
11.0	0.000	-110.530950988	-109.361602258	-1.169295006	-0.000053724	
11.0	0.001	-110.508958447	-109.361609473	-1.147298769	-0.000050205	
11.0	0.002	-110.486988407	-109.361631394	-1.125309974	-0.000047039	
11.0	0.003	-110.465040876	-109.361668024	-1.103328622	-0.000044230	0.000022181
11.5	-0.003	-110.600040798	-109.361661112	-1.238328036	-0.000051650	
11.5	-0.002	-110.576981521	-109.361624234	-1.215309469	-0.000047818	
11.5	-0.001	-110.553944704	-109.361602062	-1.192298344	-0.000044298	
11.5	0.000	-110.530930342	-109.361594596	-1.169294661	-0.000041085	

11.5	0.001	-110.507938432	-109.361601835	-1.146298419	-0.000038178	
11.5	0.002	-110.484968976	-109.361623778	-1.123309618	-0.000035580	
11.5	0.003	-110.462021979	-109.361660429	-1.100328261	-0.000033289	0.000018361
12.0	-0.003	-110.603024606	-109.361656224	-1.241327667	-0.000040715	
12.0	-0.002	-110.578965959	-109.361619379	-1.217309095	-0.000037485	
12.0	-0.001	-110.554929732	-109.361597214	-1.193297963	-0.000034555	
12.0	0.000	-110.530915919	-109.361589807	-1.169294275	-0.000031837	
12.0	0.001	-110.506924517	-109.361597076	-1.145298027	-0.000029414	
12.0	0.002	-110.482955530	-109.361619049	-1.121309220	-0.000027261	
12.0	0.003	-110.459008961	-109.361655728	-1.097327856	-0.000025377	0.000015338

T SHAPED WITH H2 HORIZONTAL						
R(bohr)	Field	Dimer Energy	N_2 Energy	H_2 Energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.542670260	-109.362004409	-1.199380145	0.018714294	
5.0	-0.002	-110.532548243	-109.361967749	-1.189367557	0.018787063	
5.0	-0.001	-110.522446990	-109.361945799	-1.179360049	0.018858858	
5.0	0.000	-110.512366419	-109.361938557	-1.169357621	0.018929759	
5.0	0.001	-110.502306685	-109.361946024	-1.159360272	0.018999611	
5.0	0.002	-110.492267587	-109.361968200	-1.149368003	0.019068616	
5.0	0.003	-110.482249168	-109.362005085	-1.139380815	0.019136732	0.000422438
6.0	-0.003	-110.564434764	-109.361845824	-1.205348070	0.002759130	
6.0	-0.002	-110.552365524	-109.361809151	-1.193335448	0.002779075	
6.0	-0.001	-110.540316895	-109.361787188	-1.181327904	0.002798197	
6.0	0.000	-110.528288867	-109.361779933	-1.169325439	0.002816505	
6.0	0.001	-110.516281432	-109.361787386	-1.157328051	0.002834005	
6.0	0.002	-110.504294581	-109.361809547	-1.145335741	0.002850707	
6.0	0.003	-110.492328308	-109.361846417	-1.133348509	0.002866618	0.000107488
7.0	-0.003	-110.572879725	-109.361776686	-1.211335818	0.000232779	
7.0	-0.002	-110.558823314	-109.361739972	-1.197323197	0.000239855	
7.0	-0.001	-110.544787420	-109.361717966	-1.183315655	0.000246201	
7.0	0.000	-110.530772040	-109.361710668	-1.169313190	0.000251818	
7.0	0.001	-110.516777170	-109.361718078	-1.155315802	0.000256710	
7.0	0.002	-110.502802804	-109.361740194	-1.141323491	0.000260881	
7.0	0.003	-110.488848944	-109.361777020	-1.127336259	0.000264335	0.000031556
8.0	-0.003	-110.579096513	-109.361718118	-1.217326304	-0.000052091	
8.0	-0.002	-110.563043584	-109.361681258	-1.201313673	-0.000048653	
8.0	-0.001	-110.547011019	-109.361659108	-1.185306122	-0.000045789	
8.0	0.000	-110.530998807	-109.361651666	-1.169303651	-0.000043490	
8.0	0.001	-110.515006955	-109.361658932	-1.153306258	-0.000041765	
8.0	0.002	-110.499035456	-109.361680905	-1.137313944	-0.000040607	
8.0	0.003	-110.483084316	-109.361717588	-1.121326710	-0.000040018	0.000012073

9.0	-0.003	-110.585041123	-109.361675313	-1.223320531	-0.000045279	
9.0	-0.002	-110.566989480	-109.361638417	-1.205307850	-0.000043213	
9.0	-0.001	-110.548958054	-109.361616229	-1.187300253	-0.000041572	
9.0	0.000	-110.530946839	-109.361608747	-1.169297740	-0.000040352	
9.0	0.001	-110.512955831	-109.361615971	-1.151300309	-0.000039551	
9.0	0.002	-110.494985037	-109.361637902	-1.133307963	-0.000039172	
9.0	0.003	-110.477034459	-109.361674540	-1.115320702	-0.000039217	0.000006062
9.5	-0.003	-110.588015940	-109.361663973	-1.226318617	-0.000033350	
9.5	-0.002	-110.568964699	-109.361627102	-1.207305919	-0.000031678	
9.5	-0.001	-110.549933617	-109.361604939	-1.188298308	-0.000030370	
9.5	0.000	-110.530922686	-109.361597481	-1.169295782	-0.000029423	
9.5	0.001	-110.511931904	-109.361604727	-1.150298343	-0.000028834	
9.5	0.002	-110.492961276	-109.361626678	-1.131305990	-0.000028608	
9.5	0.003	-110.474010806	-109.361663337	-1.112318725	-0.000028744	0.000004606
10.0	-0.003	-110.590998503	-109.361657441	-1.229317348	-0.000023714	
10.0	-0.002	-110.570947578	-109.361620602	-1.209304641	-0.000022335	
10.0	-0.001	-110.550916761	-109.361598468	-1.189297022	-0.000021271	
10.0	0.000	-110.530906046	-109.361591039	-1.169294491	-0.000020516	
10.0	0.001	-110.510915430	-109.361598313	-1.149297049	-0.000020068	
10.0	0.002	-110.490944918	-109.361620291	-1.129304696	-0.000019931	
10.0	0.003	-110.470994515	-109.361656976	-1.109317433	-0.000020106	0.000003608
10.5	-0.003	-110.593987009	-109.361653735	-1.232316571	-0.000016703	
10.5	-0.002	-110.572936336	-109.361616922	-1.211303861	-0.000015553	
10.5	-0.001	-110.551905728	-109.361594815	-1.190296242	-0.000014671	
10.5	0.000	-110.530895181	-109.361587411	-1.169293712	-0.000014058	
10.5	0.001	-110.509904692	-109.361594709	-1.148296273	-0.000013710	
10.5	0.002	-110.488934265	-109.361616711	-1.127303925	-0.000013629	
10.5	0.003	-110.467983906	-109.361653417	-1.106316670	-0.000013819	0.000002884
11.0	-0.003	-110.596979273	-109.361651333	-1.235316134	-0.000011806	
11.0	-0.002	-110.574928804	-109.361614540	-1.213303429	-0.000010835	
11.0	-0.001	-110.552898365	-109.361592452	-1.191295815	-0.000010098	
11.0	0.000	-110.530887951	-109.361585066	-1.169293293	-0.000009592	
11.0	0.001	-110.508897560	-109.361592382	-1.147295862	-0.000009316	
11.0	0.002	-110.486927196	-109.361614400	-1.125303524	-0.000009272	
11.0	0.003	-110.464976866	-109.361651123	-1.103316279	-0.000009464	0.000002342
11.5	-0.003	-110.599973708	-109.361649406	-1.238315876	-0.000008426	
11.5	-0.002	-110.576923402	-109.361612626	-1.215303177	-0.000007599	
11.5	-0.001	-110.553893096	-109.361590550	-1.192295571	-0.000006975	
11.5	0.000	-110.530882786	-109.361583177	-1.169293057	-0.000006552	

11.5	0.001	-110.507892469	-109.361590504	-1.146295634	-0.000006331	
11.5	0.002	-110.484922150	-109.361612533	-1.123303305	-0.000006312	
11.5	0.003	-110.461971834	-109.361649266	-1.100316070	-0.000006498	0.000001928
12.0	-0.003	-110.602969416	-109.361647670	-1.241315676	-0.000006070	
12.0	-0.002	-110.578919245	-109.361610899	-1.217302983	-0.000005363	
12.0	-0.001	-110.554889043	-109.361588830	-1.193295381	-0.000004832	
12.0	0.000	-110.530878813	-109.361581464	-1.169292871	-0.000004478	
12.0	0.001	-110.506888549	-109.361588797	-1.145295454	-0.000004298	
12.0	0.002	-110.482918260	-109.361610832	-1.121303131	-0.000004297	
12.0	0.003	-110.458967946	-109.361647571	-1.097315901	-0.000004474	0.000001596

The following tables are the initial data for each of the five configurations with H_2 bond length at 1.25 bohr.

LINEAR						
R(bohr)	Field	Dimer Energy	N_2 Energy	H_2 Energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.541368021	-109.362260868	-1.197477173	0.018370020	
5.0	-0.002	-110.531142569	-109.362224174	-1.187463625	0.018545230	
5.0	-0.001	-110.520939290	-109.362202188	-1.177455566	0.018718464	
5.0	0.000	-110.510758149	-109.362194908	-1.167452973	0.018889732	
5.0	0.001	-110.500599115	-109.362202336	-1.157455845	0.019059066	
5.0	0.002	-110.490462157	-109.362224470	-1.147464183	0.019226496	
5.0	0.003	-110.480347248	-109.362261312	-1.137477987	0.019392051	0.001022031
6.0	-0.003	-110.563422534	-109.361994054	-1.203448183	0.002019703	
6.0	-0.002	-110.551315226	-109.361957417	-1.191434554	0.002076745	
6.0	-0.001	-110.539229405	-109.361935491	-1.179426390	0.002132476	
6.0	0.000	-110.527165054	-109.361928275	-1.167423690	0.002186911	
6.0	0.001	-110.515122160	-109.361935768	-1.155426454	0.002240062	
6.0	0.002	-110.503100712	-109.361957970	-1.143434683	0.002291941	
6.0	0.003	-110.491100700	-109.361994883	-1.131448378	0.002342561	0.000322858
7.0	-0.003	-110.571450614	-109.361861574	-1.209412446	-0.000176594	
7.0	-0.002	-110.557376259	-109.361824946	-1.195398777	-0.000152536	
7.0	-0.001	-110.543323046	-109.361803028	-1.181390572	-0.000129446	
7.0	0.000	-110.529290968	-109.361795821	-1.167387830	-0.000107317	
7.0	0.001	-110.515280019	-109.361803319	-1.153390552	-0.000086148	
7.0	0.002	-110.501290194	-109.361825538	-1.139398737	-0.000065919	
7.0	0.003	-110.487321492	-109.361862463	-1.125412387	-0.000046642	0.000129952
8.0	-0.003	-110.577435568	-109.361783252	-1.215395331	-0.000256985	
8.0	-0.002	-110.561372597	-109.361746559	-1.199381681	-0.000244357	
8.0	-0.001	-110.545330496	-109.361724578	-1.183373495	-0.000232423	
8.0	0.000	-110.529309260	-109.361717308	-1.167370773	-0.000221179	
8.0	0.001	-110.513308888	-109.361724743	-1.151373513	-0.000210632	

8.0	0.002	-110.497329376	-109.361746899	-1.135381717	-0.000200760	
8.0	0.003	-110.481370725	-109.361783762	-1.119395386	-0.000191577	0.000065408
9.0	-0.003	-110.583279154	-109.361733802	-1.221391522	-0.000153830	
9.0	-0.002	-110.565221130	-109.361696980	-1.203377877	-0.000146273	
9.0	-0.001	-110.547183774	-109.361674869	-1.185369695	-0.000139210	
9.0	0.000	-110.529167080	-109.361667467	-1.167366977	-0.000132636	
9.0	0.001	-110.511171048	-109.361674770	-1.149369722	-0.000126556	
9.0	0.002	-110.493195677	-109.361696793	-1.131377931	-0.000120953	
9.0	0.003	-110.475240967	-109.361733520	-1.113391604	-0.000115843	0.000037987
9.5	-0.003	-110.586218501	-109.361713449	-1.224390392	-0.000114660	
9.5	-0.002	-110.567161968	-109.361676578	-1.205376751	-0.000108639	
9.5	-0.001	-110.548126025	-109.361654416	-1.186368574	-0.000103035	
9.5	0.000	-110.529110668	-109.361646963	-1.167365860	-0.000097845	
9.5	0.001	-110.510115897	-109.361654219	-1.148368610	-0.000093068	
9.5	0.002	-110.491141711	-109.361676183	-1.129376824	-0.000088704	
9.5	0.003	-110.472188110	-109.361712856	-1.110390502	-0.000084752	0.000029908
10.0	-0.003	-110.589170438	-109.361695085	-1.227389620	-0.000085733	
10.0	-0.002	-110.569115030	-109.361658180	-1.207375984	-0.000080866	
10.0	-0.001	-110.549080148	-109.361635984	-1.187367813	-0.000076351	
10.0	0.000	-110.529065790	-109.361628497	-1.167365105	-0.000072188	
10.0	0.001	-110.509071954	-109.361635717	-1.147367860	-0.000068377	
10.0	0.002	-110.489098642	-109.361657644	-1.127376080	-0.000064918	
10.0	0.003	-110.469145852	-109.361694281	-1.107389764	-0.000061807	0.000023926
10.5	-0.003	-110.592133494	-109.361679538	-1.230389176	-0.000064780	
10.5	-0.002	-110.571078957	-109.361642621	-1.209375543	-0.000060793	
10.5	-0.001	-110.550044896	-109.361620412	-1.188367374	-0.000057110	
10.5	0.000	-110.529031308	-109.361612911	-1.167364668	-0.000053729	
10.5	0.001	-110.508038190	-109.361620117	-1.146367427	-0.000050646	
10.5	0.002	-110.487065543	-109.361642029	-1.125375649	-0.000047865	
10.5	0.003	-110.466113370	-109.361678650	-1.104389337	-0.000045383	0.000019397
11.0	-0.003	-110.595106328	-109.361667907	-1.233388832	-0.000049589	
11.0	-0.002	-110.573052489	-109.361631002	-1.211375199	-0.000046288	
11.0	-0.001	-110.551019084	-109.361608806	-1.189367031	-0.000043247	
11.0	0.000	-110.529006109	-109.361601315	-1.167364326	-0.000040468	
11.0	0.001	-110.507013561	-109.361608530	-1.145367085	-0.000037946	
11.0	0.002	-110.485041443	-109.361630452	-1.123375307	-0.000035684	
11.0	0.003	-110.463089756	-109.361667081	-1.101388994	-0.000033681	0.000015908
11.5	-0.003	-110.598087235	-109.361660264	-1.236388492	-0.000038479	
11.5	-0.002	-110.575033966	-109.361623389	-1.213374857	-0.000035720	

11.5	-0.001	-110.552001095	-109.361601222	-1.190366687	-0.000033186	
11.5	0.000	-110.528988617	-109.361593759	-1.167363980	-0.000030878	
11.5	0.001	-110.505996533	-109.361601001	-1.144366737	-0.000028795	
11.5	0.002	-110.483024841	-109.361622948	-1.121374957	-0.000026936	
11.5	0.003	-110.460073547	-109.361659602	-1.098388643	-0.000025302	0.000013177
12.0	-0.003	-110.601074190	-109.361655729	-1.239388177	-0.000030284	
12.0	-0.002	-110.577021386	-109.361618890	-1.215374540	-0.000027956	
12.0	-0.001	-110.552988949	-109.361596756	-1.191366367	-0.000025826	
12.0	0.000	-110.528976877	-109.361589327	-1.167363657	-0.000023893	
12.0	0.001	-110.504985167	-109.361596600	-1.143366411	-0.000022156	
12.0	0.002	-110.481013822	-109.361618577	-1.119374628	-0.000020617	
12.0	0.003	-110.457062843	-109.361655261	-1.095388310	-0.000019272	0.000011012

T SHAPED WITH H2 HORIZONTAL						
R(bohr)	Field	Dimer Energy	N_2 Energy	H_2 Energy	Interaction Energy	Interaction Energy Range
5.0	-0.003	-110.542478866	-109.362007558	-1.197436724	0.016965416	
5.0	-0.002	-110.532385001	-109.361970908	-1.187426562	0.017012469	
5.0	-0.001	-110.522310748	-109.361948968	-1.177420516	0.017058736	
5.0	0.000	-110.512256089	-109.361941736	-1.167418584	0.017104231	
5.0	0.001	-110.502221012	-109.361949213	-1.157420767	0.017148968	
5.0	0.002	-110.492205505	-109.361971398	-1.147427066	0.017192959	
5.0	0.003	-110.482209557	-109.362008292	-1.137437479	0.017236214	0.000270798
6.0	-0.003	-110.562950075	-109.361846063	-1.203410920	0.002306908	
6.0	-0.002	-110.550890392	-109.361809388	-1.191399057	0.002318053	
6.0	-0.001	-110.538850227	-109.361787422	-1.179390280	0.002327475	
6.0	0.000	-110.526829573	-109.361780164	-1.167391111	0.002341702	
6.0	0.001	-110.514828426	-109.361787614	-1.155393306	0.002352494	
6.0	0.002	-110.502846782	-109.361809772	-1.143396140	0.002359130	
6.0	0.003	-110.490884639	-109.361846640	-1.131410034	0.002372035	0.000065127
7.0	-0.003	-110.571024305	-109.361775825	-1.209397938	0.000149458	
7.0	-0.002	-110.556972154	-109.361739106	-1.195387810	0.000154762	
7.0	-0.001	-110.542939440	-109.361717097	-1.181381795	0.000159452	
7.0	0.000	-110.528926157	-109.361709796	-1.167379893	0.000163532	
7.0	0.001	-110.514932304	-109.361717201	-1.153382104	0.000167001	
7.0	0.002	-110.500957880	-109.361739314	-1.139388426	0.000169860	
7.0	0.003	-110.487002884	-109.361776136	-1.125398861	0.000172113	0.000022655
8.0	-0.003	-110.577170091	-109.361717746	-1.215389927	-0.000062418	
8.0	-0.002	-110.561120102	-109.361680889	-1.199379767	-0.000059446	
8.0	-0.001	-110.545089417	-109.361658742	-1.183373722	-0.000056953	
8.0	0.000	-110.529078023	-109.361651302	-1.167371791	-0.000054930	
8.0	0.001	-110.513085922	-109.361658571	-1.151373974	-0.000053377	

8.0	0.002	-110.497113114	-109.361680547	-1.135380271	-0.000052296	
8.0	0.003	-110.481159600	-109.361717232	-1.119390682	-0.000051686	0.000010732
9.0	-0.003	-110.583105913	-109.361675138	-1.221385167	-0.000045608	
9.0	-0.002	-110.565056906	-109.361638244	-1.203374941	-0.000043721	
9.0	-0.001	-110.547027073	-109.361616058	-1.185368834	-0.000042181	
9.0	0.000	-110.529016411	-109.361608579	-1.167366844	-0.000040988	
9.0	0.001	-110.511024917	-109.361615805	-1.149368972	-0.000040140	
9.0	0.002	-110.493052593	-109.361637738	-1.131375217	-0.000039638	
9.0	0.003	-110.475099441	-109.361674379	-1.113385579	-0.000039483	0.000006125
9.5	-0.003	-110.586080524	-109.361663774	-1.224383543	-0.000033207	
9.5	-0.002	-110.567031864	-109.361626905	-1.205373291	-0.000031668	
9.5	-0.001	-110.548002328	-109.361604744	-1.186367160	-0.000030424	
9.5	0.000	-110.528991912	-109.361597287	-1.167365147	-0.000029478	
9.5	0.001	-110.510000616	-109.361604535	-1.148367254	-0.000028827	
9.5	0.002	-110.491028440	-109.361626488	-1.129373480	-0.000028472	
9.5	0.003	-110.472075386	-109.361663148	-1.110383825	-0.000028413	0.000004794
10.0	-0.003	-110.589063332	-109.361657216	-1.227382462	-0.000023654	
10.0	-0.002	-110.569014955	-109.361620378	-1.207372190	-0.000022387	
10.0	-0.001	-110.548985657	-109.361598246	-1.187366040	-0.000021371	
10.0	0.000	-110.528975438	-109.361590818	-1.167364011	-0.000020609	
10.0	0.001	-110.508984297	-109.361598093	-1.147366103	-0.000020101	
10.0	0.002	-110.489012235	-109.361620073	-1.127372316	-0.000019846	
10.0	0.003	-110.469059253	-109.361656758	-1.107382650	-0.000019845	0.000003809
10.5	-0.003	-110.592052154	-109.361653515	-1.230381817	-0.000016822	
10.5	-0.002	-110.571004001	-109.361616703	-1.209371533	-0.000015765	
10.5	-0.001	-110.549974895	-109.361594597	-1.188365372	-0.000014926	
10.5	0.000	-110.528964833	-109.361587193	-1.167363333	-0.000014307	
10.5	0.001	-110.507973813	-109.361594492	-1.146365416	-0.000013905	
10.5	0.002	-110.487001838	-109.361616494	-1.125371623	-0.000013721	
10.5	0.003	-110.466048907	-109.361653202	-1.104381953	-0.000013752	0.000003070
11.0	-0.003	-110.595044690	-109.361651148	-1.233381478	-0.000012064	
11.0	-0.002	-110.572996719	-109.361614356	-1.211371189	-0.000011174	
11.0	-0.001	-110.550967766	-109.361592268	-1.189365025	-0.000010473	
11.0	0.000	-110.528957828	-109.361584882	-1.167362983	-0.000009963	
11.0	0.001	-110.506966904	-109.361592198	-1.145365066	-0.000009640	
11.0	0.002	-110.484994995	-109.361614217	-1.123371270	-0.000009508	
11.0	0.003	-110.463042104	-109.361650940	-1.101381601	-0.000009563	0.000002501
11.5	-0.003	-110.598039335	-109.361649267	-1.236381305	-0.000008763	
11.5	-0.002	-110.574991511	-109.361612488	-1.213371016	-0.000008007	

11.5	-0.001	-110.551962680	-109.361590412	-1.190364851	-0.000007417	
11.5	0.000	-110.528952839	-109.361583038	-1.167362810	-0.000006991	
11.5	0.001	-110.505961989	-109.361590365	-1.144364893	-0.000006731	
11.5	0.002	-110.482990128	-109.361612395	-1.121371100	-0.000006633	
11.5	0.003	-110.460037262	-109.361649128	-1.098381431	-0.000006703	0.000002060
12.0	-0.003	-110.601035209	-109.361647574	-1.239381191	-0.000006444	
12.0	-0.002	-110.576987500	-109.361610803	-1.215370901	-0.000005796	
12.0	-0.001	-110.552958764	-109.361588734	-1.191364735	-0.000005295	
12.0	0.000	-110.528948998	-109.361581368	-1.167362694	-0.000004936	
12.0	0.001	-110.504958202	-109.361588701	-1.143364777	-0.000004724	
12.0	0.002	-110.480986375	-109.361610737	-1.119370985	-0.000004653	
12.0	0.003	-110.457033522	-109.361647475	-1.095381318	-0.000004729	0.000001715