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# Excess Valency as an Intrinsic Scale of Lewis Basicity

Joseph J. Rosmus

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EXCESS VALENCY AS AN INTRINSIC  
SCALE OF LEWIS BASICITY

A Thesis

Submitted to the Bayer School of Natural and Environmental Science

Duquesne University

In partial fulfillment of the requirements for  
the degree of Masters of Science

By

Joseph J. Rosmus

December 2013



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SCALE OF LEWIS BASICITY

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Approved November 20, 2013

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## ABSTRACT

### EXCESS VALENCY AS AN INTRINSIC SCALE OF LEWIS BASICITY

By

Joseph J. Rosmus

December 2013

Thesis supervised by Jeffrey D. Evanseck

The Lewis definition of basicity has no single reference to establish a universal order of base strength. To explore valency as an gauge of Lewis basicity, quantum mechanical calculations have been performed using the meta-hybrid density functional M06-2X with Dunning style basis sets. The electronic and thermodynamic properties of 132 isolated Lewis bases and 28 boroamine adducts have been computed. Natural bond orbital (NBO) analysis was conducted to calculate the valence population and to define the excess valency,  $EV$ , as a scale of Lewis basicity. A final equation of  $EV = -1.07(\bar{\chi}_{sub} - \chi_{donor}) + 0.74(\bar{r}_{sub} - r_{donor})$  results in a correlation of 0.87 for all investigated bases. The use of this model alleviates the confusion of multiple base scales and underscores the periodic nature of the electronic component of basicity. Combining excess valency with the double-scale equation of Drago resulted in the use of excess

valency as a means of predicting adduct bond enthalpies by  $-\Delta H = (1.25EV + .10) * E_A + C_B C_A$ .

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## LIST OF ABBREVIATIONS

EV – Excess valency of the donor atom

$\bar{\chi}_{sub}$  – average of the Pauling electronegativities for the atoms directly bound to the donor atom

$\bar{r}_{sub}$  – average of the covalent radii for the atoms directly bound to the donor atom

$E_a$  – Electrostatic term for the acid in the Drago double-scale equation

$E_b$  – Electrostatic term for the base in the Drago double-scale equation

$C_a$  – Covalent term for the acid in the Drago double-scale equation

$C_b$  – Covalent term for the base in the Drago double-scale equation

NBO – natural bond orbital program

# Chapter 1: Introduction

In 1923, Gilbert N. Lewis proposed an electronic definition of acids and bases founded on electron pair sharing.<sup>1,2</sup> While his definition is rooted in the valency of the donor and acceptor atoms, he was hesitant to use valency, as it is a quantity that cannot be directly measured by experiment. Since the inception of Lewis acid and base chemistry, many methods have been conceived to define a scale that predicts acidity and basicity.<sup>3-12</sup> Rather than predicting the ability of the acid-base pair to accept and donate electrons respectively, these methods typically use the strength of the adduct bond formed by the pair or the equilibrium constant of adduct formation to estimate acidity or basicity indirectly, despite the well-known limitations.<sup>13,14</sup>

Lewis opposed the use of the bond strength as the gauge of Lewis basicity or acidity, as factors other than the basicity are important to the adduct bond strength.<sup>2</sup> Some of these factors are orbital and steric interactions.<sup>15</sup> It is well known that using the adduct's bond strength can lead to confusing results. For instance, when comparing two acids, such as  $\text{BF}_3$  and  $\text{BH}_3$ , it is found that  $\text{BH}_3$  bonds more strongly with thioethers, while  $\text{BF}_3$  bonds more strongly with ethers.<sup>16</sup> Another instance where the use of thermodynamic data yields unexpected results is the anomalous ordering of methylated amine basicities.<sup>17</sup> As methyl groups are substituted in for hydrogens of ammonia, the basicities increase. However, the last substitution, trimethylamine, has a marked decrease in basicity.<sup>17</sup> A number of explanations have been proposed to explain the pattern of basicity in methylated amines including solvent effects,<sup>18-21</sup> steric contributions from the methyl groups,<sup>17,22</sup> and inductive effects.<sup>17-19,22-25</sup>

It is impossible to come up with a scale for Lewis basicity that does not depend on the choice of acid under the paradigm in which Lewis bases are defined by their dative bond strength. A number of these basicity scales are reviewed in the work of Laurence and Gal.<sup>26</sup> The same conundrum is true for determining the strength of the base by choosing different acids. Lewis summarized that “the relative strength depends not only upon the chosen solvent but also upon the particular base or acid used for reference.”<sup>2</sup> Laurence and Gal have summarized the data for four methods of defining Lewis base strength.<sup>26,27</sup> The first class is the *donor number* method of Olofson.<sup>28-40</sup> In this method, the strength of the adduct bond formed between the base and SbCl<sub>5</sub> in 1,2-dichloromethane is determined. The affinity of the base for SbCl<sub>5</sub> (donor number) is determined either by thermodynamic or spectroscopic methods, and is the negative of the enthalpy of formation for the Lewis adduct. A large body of the work utilizing this method has been reported on bases with a carbonyl oxygen, resulting in a very limited scale of Lewis base strength.

The second method of base strength prediction is similar to the SbCl<sub>5</sub> affinity scale but differs in that it is a BF<sub>3</sub> affinity scale. The SbCl<sub>5</sub> and BF<sub>3</sub> affinity scales correlate well as they both have a lone pair acceptor that is hard and have similar electronic and steric properties. One can transform the affinity scales by Equation 1.

$$(\text{Donor Number}) = -4.83 + 1.09(\text{BF}_3 \text{ affinity}) \quad \text{Equation 1}$$

The advantage in using the BF<sub>3</sub> affinity is that there is a larger number of bases that have been studied using the BF<sub>3</sub> affinity. However, these two methods do not always align. For example, the affinity of pyridine to SbCl<sub>5</sub> is stronger than that of triethylamine to SbCl<sub>5</sub>, while the opposite is found for BF<sub>3</sub> affinity.<sup>20,41,42</sup>

In a third class, the *equilibrium constant* is used to create a scale of basicity rather than affinity. Hydrogen bonds are a case of Lewis adducts in which the antibonding orbital of the X-H bond is the electron pair acceptor, where X is an electronegative atom. It is possible then to determine the strength of a base by analyzing changes in hydrogen-bond formation. This hydrogen-bond method has resulted in an extensive list of Lewis basicities including amines, ketones, and phenols.<sup>19,26,27,43</sup> The equilibrium constant  $K_c$  is determined from the O-H stretching frequency of the hydrogen-bond donor.<sup>19,26,27,43</sup>

The final category of basicity is a method similar to that of hydrogen bonding that has been employed for halogens. The heavy halogens, Cl, Br and I, have been shown to form weak intermolecular bonds that are similar to hydrogen-bonding, allowing halogens to act as electron pair acceptors. The halogen-bond is like the hydrogen-bond, though with greater charge transfer and dispersion interactions. The basicity scales of the hydrogen and halogen bonds do not always correlate well. For the hydrogen-bond of 4-fluorophenol, the oxygen bases are stronger than the sulfur bases while the opposite is true for the equilibrium constants with diiodine.

$$-\Delta H = E_A E_B + C_A C_B \quad \text{Equation 2}$$

A double-scale approach has been determined by Drago and Wayland that predicts the enthalpy of Lewis adduct formation using Equation 2.<sup>6</sup> The equation uses terms for the electrostatic interactions for the acid and base,  $E_A$  and  $E_B$ , as well as their propensity to form covalent bonds,  $C_A$  and  $C_B$ , in order to predict the bond dissociation enthalpy,  $\Delta H$ , of the Lewis adduct. The values of  $C_B$  and  $E_B$  were determined for a number of bases by solving a system of equations for the bases forming an adduct with  $I_2$  and phenol.<sup>6</sup>  $I_2$  was used a reference acid as a large wealth of thermodynamic data exists

for bases complexed to  $I_2$ . As a reference, a value of 1.00 was set for the  $C_A$  and  $E_A$  of  $I_2$ . It was found that the properties of  $E_B$  and  $C_B$  could be related back to the lone-pair dipole moment and total distortion polarization of the base, respectively.<sup>6</sup> Errors in this prediction method have been attributed to sterics as a comparison to the well known anomalous base strengths of Brown were investigated, giving an error of 8.2 kcal/mol for the interaction of trimethylboron with trimethylamine.<sup>6,17,22</sup>

It has previously been shown that a scale of Lewis acidity can be derived from the electronic structure of a number of primary borane compounds.<sup>44</sup> In line with Lewis' definition of acidity, it was concluded that the valency of a given acid can be correlated to the electronegativity and the covalent radii of the atoms adjacent to the electron acceptor. With current theory and technology, it is possible to calculate the electron deficiency or excess in the valence shell using computational methods.<sup>45</sup>

In order to gauge Lewis basicity as Lewis originally intended and provide a practical and universal scale of Lewis basicity, the valencies of 132 isolated Lewis bases and 28 Lewis adducts have been analyzed. Bases were selected to probe possible periodic trends of Lewis basicity by including compounds from Periods 2, 3 and 4 of Groups 14, 16, and 17 from the periodic table. Periodic trends have been assessed for the bases based upon the average substituent properties. Mono-, di-, and trisubstituted amines have been investigated, as well as substituted ethers, thioethers, and phosphines. The ability of a base to donate electrons is gauged by the excess valency, as defined below, and its dependence on the atoms directly bonded to the donor atom. We rationalize our findings based upon the average Pauling electronegativity<sup>46,47</sup> and covalent radii<sup>48</sup> of the atom

directly bound to the donor atom. This work gives new insight into the ability to compare the relative basicity of systems without the complicating steric effects.

## Chapter 2: Computational methods

Resources at the Center for Computational Sciences at Duquesne University and the Gaussian 09 program<sup>49</sup> have been used for all the electronic structure calculations. Full geometry optimizations were carried out. Density functional theory (DFT) and Moller-Plesset second-order perturbation theory (MP2)<sup>50</sup> were used to approximate the Schrödinger equation and to model the coordinate covalent bond accurately. Density functional calculations were carried out using Zhao and Truhlar's hybrid meta-generalized gradient exchange correlation functionals (M06-2X). It has been shown in the

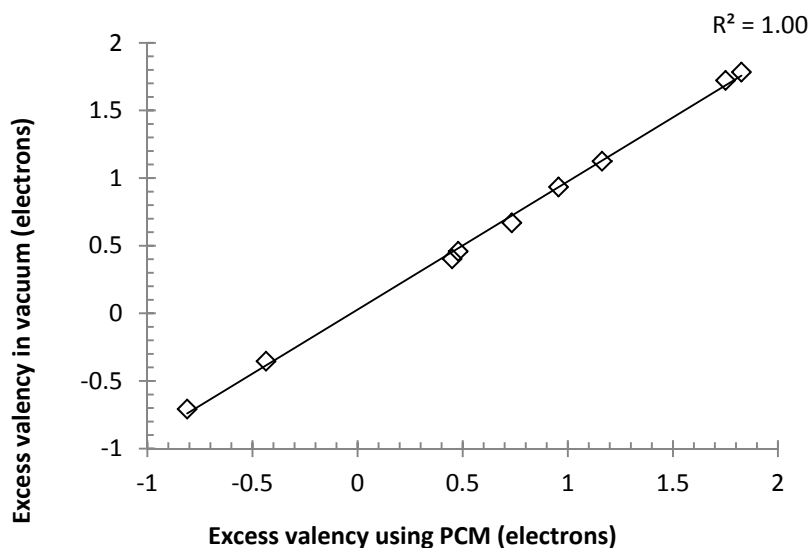


Figure 1. Comparison excess valency of tri-substituted amines for vacuum and implicitly solvated calculations

literature that M06-2X along with the Pople-style 6-311++G(3df,2p) basis set gives results comparable to those found using correlated post-SCF methods.<sup>44,51,52</sup> The systems evaluated include  $\text{BH}_3\text{NX}_n\text{H}_{(3-n)}$  and  $\text{NX}_n\text{H}_{(3-n)}$  ( $\text{X}=\text{CH}_3, \text{SiH}_3, \text{GeH}_3, \text{OH}, \text{SH}, \text{SeH}, \text{F}$ ,

Cl, and Br). This set was chosen to evaluate the effects of changing the substituent identities while being able to monitor periodic trends as these substituents all fall within the p-block of the periodic table. Changing the number of substituents allows for a larger set of data, as well as a means of investigating the effects that changing the degree of substitution has on valency. We have also investigated OXH, OX<sub>2</sub>, SXH, SX<sub>2</sub>, PXH<sub>2</sub>, PX<sub>2</sub>H, PX<sub>3</sub> (X=CH<sub>3</sub>, SiH<sub>3</sub>, GeH<sub>3</sub>, OH, SH, SeH, F, Cl, and Br) to expand our understanding of basicity from the donor identities to include the donor identities as well. For all of these systems the average Pauling electronegativity,  $\bar{\chi}_{sub}$ , and the average covalent radius,  $\bar{r}_{sub}$ , were determined. In order to do this the average of the values for the atom directly bound to the donor were taken. For example, for NCH<sub>3</sub>H<sub>2</sub>,  $\bar{\chi}_{sub}$ =2.32 as it is the average of 2.55, 2.20, and 2.20 for the carbon and 2 hydrogen, respectively. The generated data was used to illustrate how a predictive model developed using the above amine system can be used for a varying number of bases. Geometry optimizations were performed using M06-2X/6-311++G(3df,2p) for all structures.<sup>53-61</sup> These geometries were then validated as minima and thermodynamic properties were calculated



using a frequency analysis.<sup>62</sup> All calculated molecular energies were corrected for basis set superposition error using the counterpoise method of Boys and Bernardi<sup>63</sup> as well as the PCM model<sup>64,65</sup> to apply implicit water solvation (Figure 1). The results obtained from MP2 calculations verified that the more computationally expedient DFT calculations were sufficient, as the error in excess valency was approximately 0.1 electrons for 28 bases of the form  $NX_nH_{(3-n)}$  studied (Figure 2).

Natural bond orbital (NBO) analysis<sup>66-69</sup> was performed using the NBO 5.9 program,<sup>45</sup> embedded within the Gaussian 09 suite. NBO transforms the non-orthogonal atomic orbitals from the HF wave function into orthonormal natural atomic orbitals

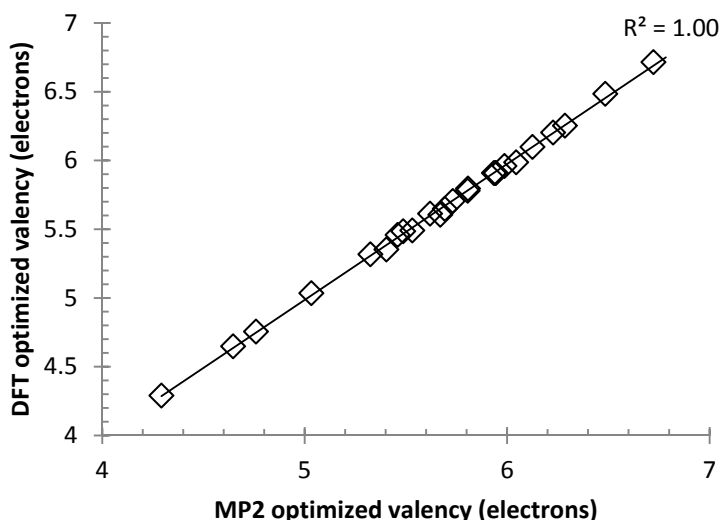


Figure 2. Comparison excess valency of tri-substituted amines DFT and MP2 calculations.

(NAO),<sup>70</sup> natural hybrid orbitals (NHO),<sup>71</sup> natural bond orbitals (NBO)<sup>66</sup> and natural localized molecular orbitals (NLMO).<sup>72</sup> This allows electron density to be treated in a more intuitive manner, *i.e.* localized onto bonds, atoms, and lone pairs, leading to the best possible description of the molecule as a localized Lewis structure. NBO gives the energy

involved in specific orbital interactions. HF/aug-cc-pVQZ level of theory was used for all NBO calculations, since the combination has been shown to provide accurate orbital predictions.<sup>73</sup> NBO was used to determine the excess valency of the donor atoms as a gauge of Lewis basicity. The correlations of the excess valency and the electronegativity or radii was found using linear regression and the combined correlation of electronegativity and covalent radii with excess valency was determined using the method of multiple regression analysis.

### 3 Development of predictive model for evaluating Lewis basicity

#### basicity

The excess valency of nitrogen has been calculated to investigate the periodic causes of Lewis basicity in three stages. The first stage was to investigate electronegativity and radius of amine substituents and how they affect the excess valency, where the donor atom was taken to be a tertiary nitrogen. The three substituents on the nitrogen were varied asymmetrically and symmetrically. The substituents were chosen to highlight periodicity and electron donating/withdrawing power. The second step was to model the trend of valency with the electronegativity and radii of the substituent atoms, which would allow for the quick determination of Lewis base strength without the need for high-level computations or costly experiments. The third and final step was to

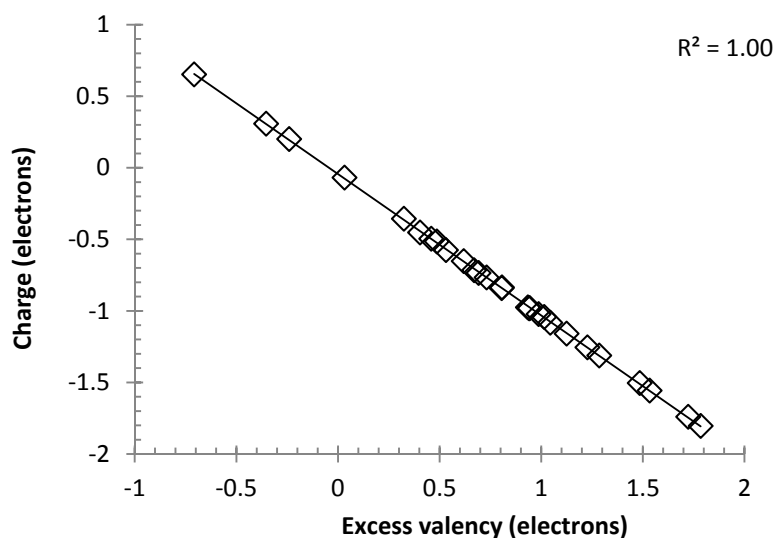


Figure 3. Comparison for excess valency of substituted amines with the charge

calculate thermodynamic properties and electronic properties of the base and compare how the properties correspond with existing scales of Lewis basicity in the literature. In particular, the electronic parameter of the Drago double-scale equation was replaced with the excess valency in order to predict the Lewis adduct bond strength.

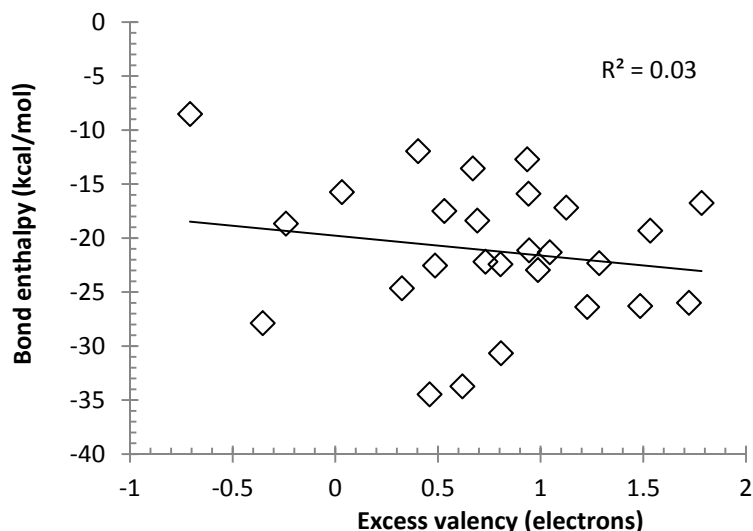


Figure 4. Bond enthalpy of  $\text{BH}_3\text{NH}_{(3-n)}\text{X}_n$  compared with the excess valency of the isolated base.

The nucleophilicity, and thus the basicity of the bases, is considered in terms of the excess of the valence population. This excess is determined by subtracting the formal valency of the donor atom from the calculated valence population from NBO. As expected, the atomic charge and the excess valency are highly correlated ( $R^2=1.00$  in Figure 3). This indicates that the charge and valency both similarly reflect the degree of Lewis basicity. However, the excess valency of nitrogen and the binding enthalpy are not well correlated ( $R^2=0.03$  in Figure 4). This poor correlation highlights the need for a new paradigm in understanding and predicting Lewis basicity.

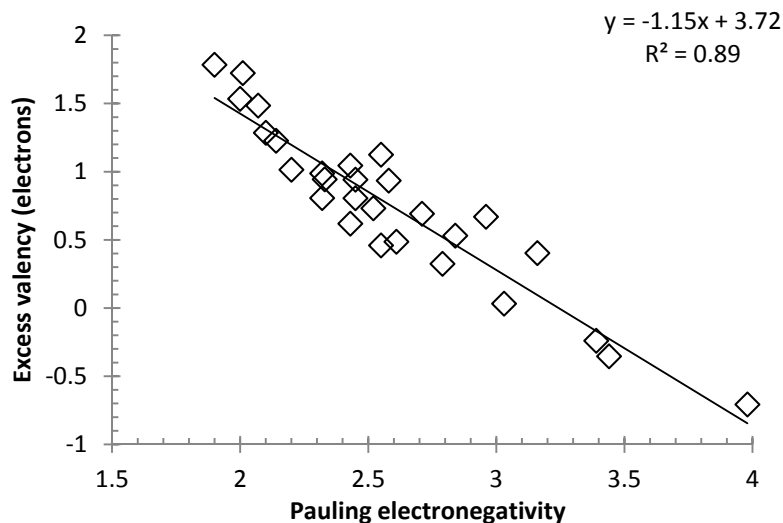


Figure 5. Correlation for excess valency of the nitrogen of 28 isolated amines with average Pauling Electronegativity of the atom bound to the nitrogen

The average substituent electronegativity,  $\bar{\chi}_{sub}$ , is estimated as a third of the sum of the Pauling electronegativities of the atoms bound directly to the donor atom. Considering all 28 amine bases, a strong correlation is seen with  $\bar{\chi}_{sub}$  ( $R^2=0.88$  Figure 5). These results indicate that as substituents become more electronegative, the excess valency of the donor atom decreases, yielding a weaker Lewis base. However, the radii,  $\bar{r}_{sub}$ , correlate poorly with the excess valency of the amines ( $R^2=0.20$  Figure 6). The correlation coefficients for  $\bar{\chi}_{sub}$  and  $\bar{r}_{sub}$  suggests that the substituent electronegativity of amine bases accounts for 68% more of the observed variance in valency than the substituent radii does.

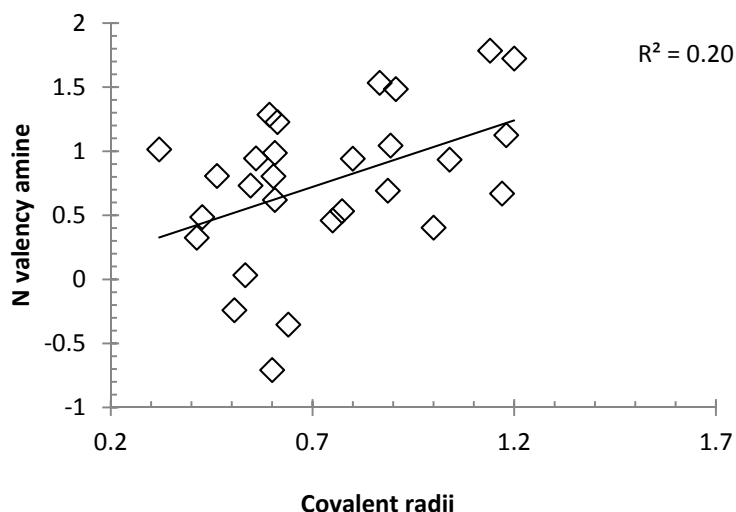


Figure 6. Correlation between the excess valency of the nitrogen for 28 isolated amines and the average radii of the atoms bound to the nitrogen.

When second period amines ( $\text{NH}_{3-n}(\text{CH}_3)_n$ ,  $\text{NH}_{3-n}(\text{OH})_n$ ,  $\text{NH}_{3-n}\text{F}_n$ ) are considered, excess valency and  $\bar{\chi}_{sub}$  are highly correlated ( $R^2=0.99$ ) while excess valency and  $\bar{r}_{sub}$  are poorly correlated ( $R^2=0.05$ ). For third period amines ( $\text{NH}_{3-n}(\text{SiH}_3)_n$ ,  $\text{NH}_{3-n}(\text{SH})_n$ ,  $\text{NH}_{3-n}\text{Cl}_n$ ), the correlation of excess valency and electronegativity lowers slightly ( $R^2=0.90$ ) and excess valency and radii continues to be low ( $R^2=0.06$ ). Evaluating the effects on fourth period substituents ( $\text{NH}_{3-n}(\text{GeH}_3)_n$ ,  $\text{NH}_{3-n}(\text{SeH})_n$ ,  $\text{NH}_{3-n}\text{Br}_n$ ) yields a moderate correlation between excess valency and electronegativity ( $R^2=0.77$ ) while the correlation between excess valency and radii remains the same as for the previous period ( $R^2=0.06$ ). These findings are consistent with the Brønsted-Lowry approach to acidity where electronegativity explains the variation in acid strength within the same period.

Similar to the results of moving across a period, a moderate to high correlation between excess valency and electronegativity is observed when going down group 14 ( $\text{NH}_{3-n}(\text{CH}_3)_n$ ,  $\text{NH}_{3-n}(\text{SiH}_3)_n$ ,  $\text{NH}_{3-n}(\text{GeH}_3)_n$ ) ( $R^2=0.97$ ), group 16 ( $\text{NH}_{3-n}(\text{OH})_n$ ,  $\text{NH}_{3-n}$

$n(\text{SH})_n$ ,  $\text{NH}_{3-n}(\text{SeH})_n$  ( $R^2=0.88$ ), and group 17 ( $\text{NH}_{3-n}\text{F}_n$ ,  $\text{NH}_{3-n}\text{Cl}_n$ ,  $\text{NH}_{3-n}\text{Br}_n$ ) ( $R^2=0.88$ ).

Correlation with covalent radii is significantly improved going down groups as opposed to across periods with coefficients of determination for excess valency and radii being of  $R^2=0.54$ ,  $R^2=0.28$ , and  $R^2=0.13$  for groups 14, 16, and 17, respectively. In future work, group 15 substituents will be considered. However, due to complications with the computations, these results are not presented herein. These complications arise from reorientation of the molecules to attain an energy minimized structure.

While excess valency and substituent electronegativity are highly correlated, improved correlation has been obtained by correlating the average of both the electronegativity and of the radii of the atoms coordinated to the donor atom. This has been achieved by the method of multiple regression analysis with independent variables being the average electronegativity,  $\bar{\chi}_{sub}$ , and covalent radii,  $\bar{r}_{sub}$ , of the atoms directly adjacent to the nitrogen donor, and a dependent excess valency, EV, which can be calculated using Equation 3.

$$EV = b + m_1\bar{\chi}_{sub} + m_2\bar{r}_{sub} \quad \text{Equation 3}$$

Here  $b$  is the intercept,  $m_1$  and  $m_2$  are the coefficients for the electronegativity and radii, respectively. The values for the coefficients, intercepts and correlation are given in Table 1. As can be seen in Table 2, the correlations obtained from using this method are improved over both the correlations of electronegativity and radii. The negative value of  $b$  is attributed to the fact that the electronegativity draws electrons from nitrogen resulting in a lower excess valency. The radii results in a greater overlap of orbitals that can be attributed to a higher valence population in the donor atom.

Table 1. Coefficients and intercepts for equation 3 for all amine data as well as for the data in the various groups

	$m_1$	$m_2$	$b$	$R^2$
All	-1.07	0.74	2.98	0.97
Period 2	-1.13	0.98	3.02	0.99
Period 3	-0.98	1.19	2.38	0.99
Period 4	-0.87	1.30	1.84	0.99
Group 14	-0.90	-0.28	2.95	0.99
Group 16	-1.08	0.62	3.12	0.99
Group 17	-1.14	0.69	3.21	0.99

Table 2. Correlation coefficients for linear combinations of electronegativity and radii with the basicity of the nitrogen.

	$\bar{\chi}_{sub} - R^2$	$\bar{r}_{sub} - R^2$	Eq 3 - $R^2$
Group 14	0.97	0.54	0.99
Group 16	0.88	0.28	1.00
Group 17	0.88	0.13	1.00
Period 2	0.99	0.05	0.99
Period 3	0.90	0.06	0.99
Period 4	0.77	0.06	0.99
Primary	0.96	0.70	0.99
Secondary	0.94	0.74	0.99
Tertiary	0.93	0.77	0.99
All Data	0.88	0.20	0.97



## Chapter 4: Extending the valence Lewis basicity to other bases and properties

Thus far, a trend has been developed for prediction of Lewis base strength predicted by excess valency. This prediction can be performed with just the electronegativity and radii of the atoms bound to the donor atom. This trend is intrinsic as it depends only on the nature of the base and does not change with reference to a particular acid binding motif. As this trend was developed using only amine bases, it is important to test the performance of Equation 3 against other donors.

In order to show this, 4 different centers were investigated. The trend developed for amines, in which electronegativity and radii and scaled by -1.07 and 0.74, respectively, was plotted against the excess valency in order to show that the trend holds for all donor atoms. The results show that the trends predict the valency with accuracy comparable to that of the amines. These coefficients of determination were 0.97, 0.99, 0.87, and 0.80 for the N, O, P and S type donors, respectively. From this, it was possible to obtain Equation 4 by working the donor identity into Equation 3 in place of the intercept.

$$EV = -1.07(\bar{\chi}_{sub} - \chi_{donor}) + 0.74(\bar{r}_{sub} - r_{donor}) \quad \text{Equation 4}$$

This is a slight modification on Equation 3 in which it is possible to also determine the identity of the intercept for a given donor. In a comparison of the NBO calculated excess valency and that of excess valency as given by Equation 4, coefficients of determination were found to be  $R^2=0.97, 0.98, 0.80,$  and  $0.77$  for N, O, P and S type donors, respectively. It was also found that  $R^2=0.71, 0.82,$  and  $0.87$  for period 2 donors, period 3

donors and all donors, respectively. Using Equation 4, it is possible to determine the Lewis basicity that will account for variance in the substituents as well as the donor atom.

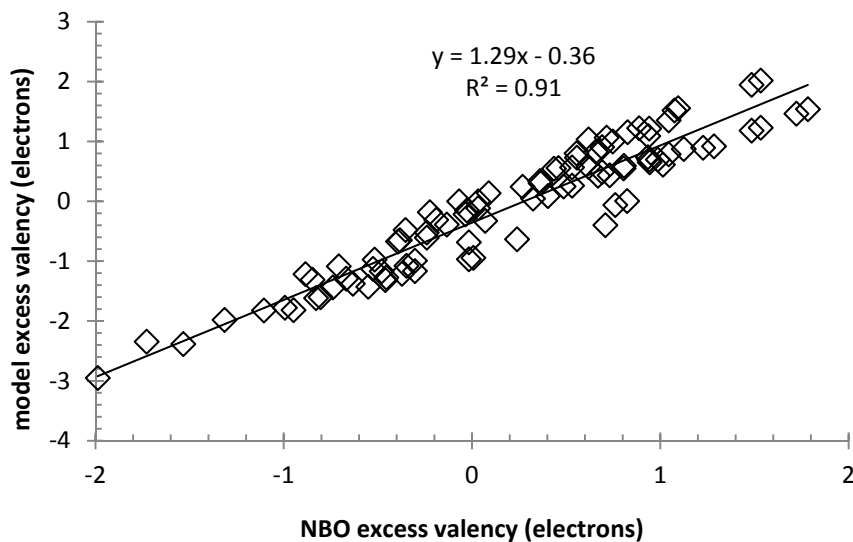


Figure 7. Comparison between the NBO calculated excess valency and that calculated using Equation 4

At face value, the biggest criticism one could make would be that the model developed herein only attributes changes in basicity to the atom bound directly to the donor. For instance, it is known that the affinity of the I<sub>2</sub> halogen bond for primary amines increases as the carbon chain increase in size from 20.1 for ammonia to 35.1 for n-butylamine.<sup>26,74</sup> It would then be expected that this same behavior would be true for the electronic basicity as well. The valency was calculated using NBO for molecules of the form NXH<sub>2</sub> (X=methoxy, cyano, ethyl, propyl and butyl groups as well as a benzyl group with the following substituents on the ring p-Br, p-CH<sub>3</sub>, p-Cl, p-F, p-H, p-OH, m-Cl, p-CH<sub>2</sub>CH<sub>3</sub>, p-CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>, p-OCH<sub>3</sub>, and p-OCH<sub>2</sub>CH<sub>3</sub>). The data is given in Figure 8 for this investigation. All of the data points shown are the NBO calculated excess valencies for primary amines. The lines represent the amines investigated in Chapter 3 with excess

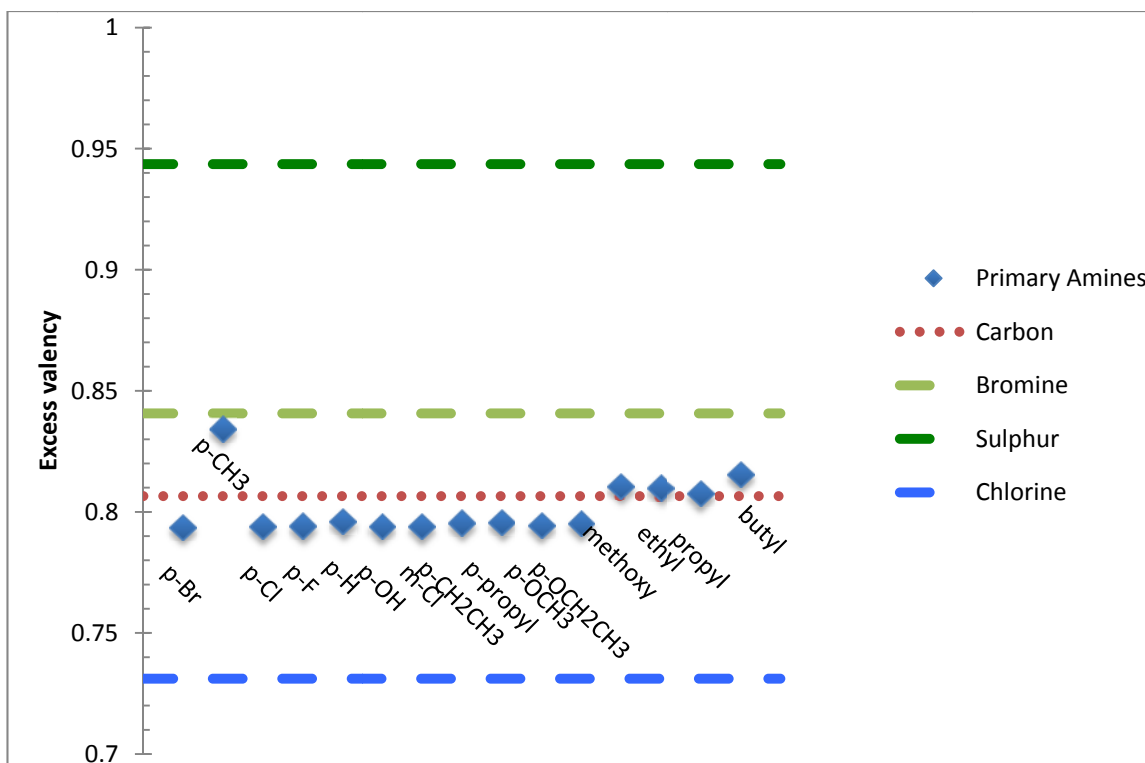


Figure 8. Investigation of primary amines where the atoms directly bound to the nitrogen are held constant and the variation is seen beyond the carbon. Lines shown represent the bases investigated in Chapter 3 with a valency closest to those investigated herein.

valency closest to the data in Figure 8. The results of this investigation were that for the electronic basicity expressed by excess valency, the variation is limited to the atom directly bound to the nitrogen. The calculated excess valency ranged from 0.842 to 0.794 for  $\text{NH}_2\text{CN}$  and  $\text{NH}_2\text{C}_6\text{H}_4\text{Br}$ , respectively. The variation in excess valency when the bound atoms were varied resulted in a maximum of 1.784 for  $\text{N}(\text{SiH}_3)_3$  and a minimum of -0.707 for  $\text{NF}_3$ . This is contrary to the effective expected from evaluation of the experimental affinities and suggests that the inductive effect is not important to the electronic basicity of a molecule.

Existing scales of Lewis basicity suffer from definitions that do not capture the nature of the valence of the base but rather depend on the binding of the base to a particular acid.

This leads to the need to investigate each base with the particular acid in order to know its basicity. Our model remedies both of these issues. However, for a model to be acceptable it must be a useful prediction tool. Chemical intuition allows us to know that for most base scales, the weaker bases should have strongly electron withdrawing groups bound to the donor. This is in line with our model as well as the scales of amine basicity outlined elsewhere.<sup>75</sup>

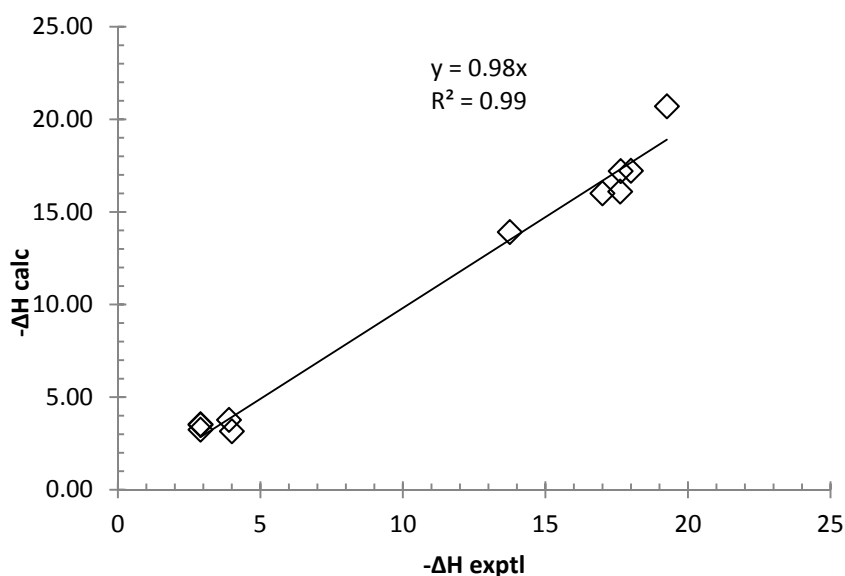


Figure 9. A straight line is realized when the bond enthalpy is calculated by equation 5 is plotted against the bond enthalpy from experiment. The lower cluster belongs to the bases complexed to  $I_2$  and the higher to those complexed with  $B(CH_3)_3$

Equation 2 gives the double-scale equation for predicting enthalpy of interaction for Lewis adducts. The results have been shown to correlate well for a number of acids and bases.<sup>6</sup> The values published for  $E_B$  correlate well with the excess valency reported here. The means of converting excess valency to a usable value for use in Equation 2 was performed by a least-squared fitting between  $E_B$  and EV and resulted in an equation of  $E_B=1.25*EV+0.10$ . By using the values of  $E_A$ ,  $C_A$ , and  $C_B$  reported,<sup>6</sup> it becomes possible

to use Equation 5 to predict Lewis adduct enthalpies with accuracy as can be seen in Figure 9. Results of this scaling of EV to fit  $E_B$  are given in Table 2 as well as the enthalpies resulting from the Equation 5. The reason that EV replacement for  $E_B$  results

$$-\Delta H = (1.25 * EV + .10) * E_A + C_B C_A \quad \text{Equation 5}$$

in agreeable enthalpies is a consequence of the description for  $E_B$  given by Drago that  $E_B$  is related to the dipole moment. A higher population of the donor will result in a greater dipole moment as more electron density is located on the negative end of the dipole.

Table 2. Comparison of excess valency and double scale equation. Scaled excess valency is the parenthetical term of Equation 5 and the  $-\Delta H_{calc}$  is the value calculated from the use of Equation 5. The starred values are corrected with the steric contribution.

Acid	Base	$E_B^6$	Scaled excess valency	$-\Delta H_{exptl}$ (kcal/mol)	$-\Delta H_{calc}$ (kcal/mol)
B(CH <sub>3</sub> ) <sub>3</sub>	NH <sub>3</sub>	1.34	1.37	13.7 <sup>22</sup>	13.8
B(CH <sub>3</sub> ) <sub>3</sub>	NH <sub>2</sub> CH <sub>3</sub>	1.19	1.11	17.6 <sup>22</sup>	17.7
B(CH <sub>3</sub> ) <sub>3</sub>	NH(CH <sub>3</sub> ) <sub>2</sub>	0.94	0.87	19.3 <sup>22</sup>	20.7*
B(CH <sub>3</sub> ) <sub>3</sub>	N(CH <sub>3</sub> ) <sub>3</sub>	0.59	0.67	17.6 <sup>22</sup>	23.8*
B(CH <sub>3</sub> ) <sub>3</sub>	NH <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )	1.26	1.11	18.0 <sup>22</sup>	18.1
B(CH <sub>3</sub> ) <sub>3</sub>	NC <sub>5</sub> H <sub>5</sub>	0.88	0.66	17.0 <sup>76</sup>	17.3
(CH <sub>3</sub> ) <sub>3</sub> COH	O(CH <sub>2</sub> ) <sub>4</sub>	0.61	0.81	2.9 <sup>77</sup>	3.5
(CH <sub>3</sub> ) <sub>3</sub> COH	NC <sub>5</sub> H <sub>5</sub>	0.88	0.66	4.0 <sup>77</sup>	3.2
(CH <sub>3</sub> ) <sub>3</sub> COH	CO(CH <sub>3</sub> ) <sub>2</sub>	0.706	0.84	2.9 <sup>77</sup>	3.2
(CH <sub>3</sub> ) <sub>3</sub> COH	CH <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub>	0.639	0.88	2.9 <sup>77</sup>	3.5
(CH <sub>3</sub> ) <sub>3</sub> COH	HCON(CH <sub>3</sub> ) <sub>3</sub>	0.97	0.93	3.9 <sup>77</sup>	3.8

As a result of being based upon the double-scale equation of Drago, Equation 5 suffers the same errors. Namely, this method is unable to predict the affinity for a system that is highly dependent upon the sterics. To correct for this, the steric energy must be known and added to the results of equation 5. This has been done for the starred values in Table 2.

## Chapter 5: Conclusion

A predictive trend has been developed from 28 amines for predicting Lewis basicity from excess valency. This is an important advancement in the field of Lewis basicity as it allows for a back of the envelope method of determining intrinsic Lewis basicity regardless of the Lewis acid being used to form an adduct bond. This also allows Lewis basicity to be defined using the principles set forth by Gilbert Lewis. Lewis basicity is predominantly determined by the electronegativity of the atoms directly bound to the donor atom and is somewhat dependent on the radii of the bound atoms. Furthermore, not only can the valency be used as a correct scale of the basicity but it also can be used a predictive tool for the bond enthalpies of Lewis adduct formation.

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## Supplemental Information

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-----  
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Sum of electronic and thermal Energies=	-2656.661741
Sum of electronic and thermal Enthalpies=	-2656.660797
Sum of electronic and thermal Free Energies=	-2656.693870

NImag=0

Br1H2N1

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H,1,r4,2,a4,3,d4,0

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a3=104.28643923  
a4=104.28643923  
d4=110.90480881

--- Geometry Optimization ---

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[SG(Br1N1),X(H2)]\@

--- NBO Single Point ---

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HF=-2630.0876504

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NImag=0	

B1Br2H4N1

-----  
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H,1,r5,2,a5,3,d5,0  
Br,2,r6,1,a6,3,d6,0  
Br,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0

r2=1.64484391  
r3=1.20366467  
r4=1.2038696  
r5=1.19754662  
r6=1.89424949  
r7=1.8942087  
r8=1.01840998  
a3=101.84754918  
a4=101.91795494  
a5=105.72541506  
a6=113.63721026  
a7=113.6434668  
a8=109.15936003  
d4=118.88043161  
d5=239.52180863  
d6=184.46794083

d7=56.04038207  
d8=300.24604162

--- Geometry Optimization ---

```
1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\B1Br2H4N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p)
opt=(z-matrix,noeigen) optcyc=100 freq
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Br,2,
r6,1,a6,3,d6,0\Br,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\r2=1.64484391\r3=1.20366467\r4=
1.2038696\r5=1.19754662\r6=1.89424949\r7=1.8942087\r8=1.01840998\a3=101.847549
18\a4=101.91795494\a5=105.72541506\a6=113.63721026\a7=113.6434668\a8=109.159
36003\d4=118.88043161\d5=239.52180863\d6=184.46794083\d7=56.04038207\d8=300.
24604162\Version=EM64M-G09RevC.01\State=1-A\HF=-
5203.6243702\RMSD=4.941e-09\RMSF=8.866e-05\Dipole=0.0826609,-
0.1417087,1.4686182\Quadrupole=3.2299465,2.5991503,-
5.8290968,0.5584229,0.6193943,-1.0593927\PG=C01 [X(B1Br2H4N1)]\@
```

--- NBO Single Point ---

```
1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1Br2H4N1\ROSMUSJ\18-Jun-
2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read
geom=allcheck\title\0,1\B\N,1,1.6448439107\H,1,1.2036646705,2,101.84754918\H,1,1.
2038695961,2,101.91795494,3,118.88043161,0\H,1,1.1975466151,2,105.72541506,3,23
9.52180863,0\Br,2,1.8942494889,1,113.63721026,3,184.46794083,0\Br,2,1.8942087026
,1,113.6434668,3,56.04038207,0\H,2,1.0184099801,1,109.15936003,3,300.24604162,0\
Version=EM64M-G09RevC.01\State=1-A\HF=-5226.3215476\RMSD=5.154e-
09\Dipole=0.0769364,-0.132088,1.6007917\Quadrupole=3.4619794,2.7920937,-
6.254073,0.5929429,0.7226999,-1.2356308\PG=C01 [X(B1Br2H4N1)]\@
```

HF=-5203.6243702

Sum of electronic and zero-point Energies=	-5230.206918
Sum of electronic and thermal Energies=	-5230.201430
Sum of electronic and thermal Enthalpies=	-5230.200486
Sum of electronic and thermal Free Energies=	-5230.237981

NImag=0

Br2H1N1

-----

0,1

N

Br,1,r2

Br,1,r3,2,a3

H,1,r4,2,a4,3,d4,0

r2=1.88899052

r3=1.88870978

r4=1.01832831  
a3=111.84798549  
a4=102.66941396  
d4=109.35581734

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\Br2H1N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Br,1,r2\Br,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.88899052\r3=1.88870978\r4=1.01832831\a3=111.84798549\a4=102.66941396\d4=109.35581734\Version=EM64M-G09RevC.01\State=1-A\HF=-5203.6244958\RMSD=4.720e-09\RMSF=5.629e-05\Dipole=-0.0925174,-0.4594425,-0.0627869\Quadrupole=0.1413325,-0.5447939,0.4034614,1.5624642,-0.3240332,1.0578819\PG=C01 [X(Br2H1N1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\Br2H1N1\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Br,1,1.888990517\Br,1,1.8887097832,2,111.84798549\H,1,1.0183283147,2,102.66941396,3,109.35581734,0\Version=EM64M-G09RevC.01\State=1-A\HF=-5199.9061025\RMSD=5.248e-09\Dipole=-0.0906627,-0.4924691,-0.0614357\Quadrupole=0.1274096,-0.4786147,0.3512051,1.5652297,-0.2760087,1.059847\PG=C01 [X(Br2H1N1)]\@

HF=-5203.6244958

Sum of electronic and zero-point Energies=	-5203.608253
Sum of electronic and thermal Energies=	-5203.604462
Sum of electronic and thermal Enthalpies=	-5203.603518
Sum of electronic and thermal Free Energies=	-5203.637234
NImag=0	

B1Br3H3N1

-----  
0,1  
B  
N,1,rN  
H,1,rH,2,aH  
H,1,rH,2,aH,3,-120.,0  
H,1,rH,2,aH,3,120.,0  
Br,2,rB,1,aB,3,180.,0  
Br,2,rB,1,aB,3,60.,0  
Br,2,rB,1,aB,3,-60.,0

rN=1.68395794  
rH=1.19929251  
rB=1.90620376

aH=102.21922343  
aB=110.19931492

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1Br3H3N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,rN\H,1,rH,2,aH\H,1,rH,2,aH,3,-  
120.,0\H,1,rH,2,aH,3,120.,0\Br,2,rB,1,aB,3,180.,0\Br,2,rB,1,aB,3,60.,0\Br,2,rB,1,aB,3,-  
60.,0\rN=1.68395794\rH=1.19929251\rB=1.90620376\aH=102.21922343\aB=110.1993  
1492\Version=EM64M-G09RevC.01\State=1-A1\HF=-7777.1577127\RMSD=6.146e-  
09\RMSF=3.610e-05\Dipole=0.,0.,1.3383243\Quadrupole=3.1182785,3.1182785,-  
6.236557,0.,0.,0.\PG=C03V [C3(N1B1),3SGV(Br1H1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\B1Br3H3N1\ROSMUSJ\18-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6839579436\H,1,1.1992925112,2,102.21922343\H,1,1.  
1992925112,2,102.21922343,3,-  
120.,0\H,1,1.1992925112,2,102.21922343,3,120.,0\Br,2,1.9062037595,1,110.19931492,  
3,180.,0\Br,2,1.9062037595,1,110.19931492,3,60.,0\Br,2,1.9062037595,1,110.19931492  
,3,-60.,0\Version=EM64M-G09RevC.01\State=1-A1\HF=-  
7798.1431016\RMSD=4.324e-  
09\Dipole=0.,0.,1.4708196\Quadrupole=3.3436614,3.3436614,-  
6.6873228,0.,0.,0.\PG=C03V [C3(N1B1),3SGV(Br1H1)]\@

HF=-7777.1577127

Sum of electronic and zero-point Energies= -7803.743509  
Sum of electronic and thermal Energies= -7803.736622  
Sum of electronic and thermal Enthalpies= -7803.735678  
Sum of electronic and thermal Free Energies= -7803.776186  
NImag=0

Br3N1

-----  
0,1  
N  
Br,1,r2  
Br,1,r3,2,a3  
Br,1,r4,2,a4,3,d4,0

r2=1.89977744  
r3=1.89943903  
r4=1.89943901  
a3=109.23585892

a4=109.23585877  
d4=119.47998203

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\POpt\RM062X\6-311++G(3df,2p)\Br3N1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Br,1,r2\Br,1,r3,2,a3\Br,1,r4,2,a4,3,d4,0\r2=1.89977744\r3=1.89943903\r4=1.89943901\ a3=109.23585892\ a4=109.23585877\ d4=119.47998203\Version=EM64M-G09RevC.01\State=1-A\HF=-7777.1577831\RMSD=2.465e-09\RMSF=6.535e-05\Dipole=0.0994324,-0.1704311,0.0695816\Quadrupole=0.3727198,-1.1285237,0.7558039,1.327804,-0.5470245,0.9376196\PG=C01 [X(Br3N1)]\@\

--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\Br3N1\ROSMUSJ\18-Jun-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Br,1,1.8997774372\Br,1,1.8994390277,2,109.23585892\Br,1,1.8994390111,2,109.23585877,3,119.47998203,0\Version=EM64M-G09RevC.01\State=1-A\HF=-7771.737141\RMSD=7.310e-09\Dipole=0.1204681,-0.2064872,0.0854098\Quadrupole=0.3726728,-1.1248284,0.7521556,1.3244917,-0.5477432,0.9388538\PG=C01 [X(Br3N1)]\@\

HF=-7777.1577831

Sum of electronic and zero-point Energies=	-7777.152415
Sum of electronic and thermal Energies=	-7777.147334
Sum of electronic and thermal Enthalpies=	-7777.146390
Sum of electronic and thermal Free Energies=	-7777.184746

NImag=0

C1H8B1N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
C,2,r6,1,a6,3,d6,0  
H,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,6,r10,2,a10,1,d10,0  
H,6,r11,2,a11,1,d11,0

r2=1.63460246  
r3=1.20646339



r4=1.20623951  
r5=1.2065875  
r6=1.47417721  
r7=1.01580685  
r8=1.01583396  
r9=1.08903305  
r10=1.08650331  
r11=1.08640855  
a3=105.32158955  
a4=105.06906861  
a5=105.09543379  
a6=113.61460981  
a7=108.27757631  
a8=108.3210919  
a9=111.68889802  
a10=108.03937104  
a11=108.00587385  
d4=120.10876998  
d5=239.95567518  
d6=180.24360093  
d7=57.78165171  
d8=302.76321733  
d9=180.36115108  
d10=59.03364059  
d11=301.78556185

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-  
311++G(3df,2p)\C1H8B1N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\C,2,r  
6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d1  
0,0\H,6,r11,2,a11,1,d11,0\r2=1.63460246\r3=1.20646339\r4=1.20623951\r5=1.2065875  
\r6=1.47417721\r7=1.01580685\r8=1.01583396\r9=1.08903305\r10=1.08650331\r11=1.  
08640855\a3=105.32158955\a4=105.06906861\a5=105.09543379\a6=113.61460981\a7=  
108.27757631\a8=108.3210919\a9=111.68889802\a10=108.03937104\a11=108.0058738  
5\d4=120.10876998\d5=239.95567518\d6=180.24360093\d7=57.78165171\d8=302.7632  
1733\d9=180.36115108\d10=59.03364059\d11=301.78556185\\Version=EM64M-  
G09RevC.01\State=1-A\HF=-95.8406542\RMSD=8.055e-09\RMSF=1.063e-04\Dipole=-  
0.1084698,-0.0007852,2.0480392\Quadrupole=1.35977,1.1757983,-  
2.5355682,0.0017418,1.761234,0.0059322\PG=C01 [X(C1H8B1N1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\C1H8B1N1\ROSMUSJ\15-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6344695953\H,1,1.2065742322,2,105.3402816\H,1,1.2  
064287194,2,105.05457064,3,120.09490643,0\H,1,1.2069023488,2,105.07950148,3,239.

95870666,0\C,2,1.4742036272,1,113.61742543,3,180.243387,0\H,2,1.0158565015,1,108.27281106,3,57.78398854,0\H,2,1.0158712568,1,108.31666229,3,302.76004205,0\H,6,1.0890279362,2,111.69178288,1,180.36138761,0\H,6,1.0865155093,2,108.03679048,1,59.03603427,0\H,6,1.0864394692,2,108.00548648,1,301.78431645,0\\Version=EM64M-G09RevC.01\State=1-A\HF=-121.7019484\RMSD=4.030e-09\Dipole=-0.1096551,-0.0008787,2.1160706\Quadrupole=1.4014613,1.2612739,-2.6627353,0.0013732,1.8688977,0.0069493\PG=C01 [X(C1H8B1N1)]\@

HF=-95.8406542

Sum of electronic and zero-point Energies= -122.394794  
Sum of electronic and thermal Energies= -122.390023  
Sum of electronic and thermal Enthalpies= -122.389079  
Sum of electronic and thermal Free Energies= -122.420706  
NImag=0

C1H5N1

-----

0,1  
N  
C,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.46020973  
r3=1.01189427  
r4=1.01189499  
a3=110.65031695  
a4=110.65398095  
d4=118.0749232  
r5=1.095172  
r6=1.08919337  
r7=1.08918054  
a5=114.8201245  
a6=109.15702172  
a7=109.15157491  
d5=59.0182916  
d6=-62.49154993  
d7=180.52082991

--- Geometry Optimization ---

```

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\C1H5N1\ROSMUSJ\14-
Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\N\C,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6
,0\H,2,r7,1,a7,4,d7,0\r2=1.46020973\r3=1.01189427\r4=1.01189499\a3=110.65031695\
a4=110.65398095\d4=118.0749232\r5=1.095172\r6=1.08919337\r7=1.08918054\a5=114
.8201245\a6=109.15702172\a7=109.15157491\d5=59.0182916\d6=-
62.49154993\d7=180.52082991\Version=EM64M-G09RevC.01\State=1-A\HF=-
95.8412109\RMSD=9.281e-09\RMSF=2.445e-05\Dipole=0.2579585,-
0.4299102,0.1534109\Quadrupole=0.563438,-0.3048287,-0.2586093,0.8137611,-
0.8174526,1.3626795\PG=C01 [X(C1H5N1)]\@
--- NBO Single Point ---
1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\C1H5N1\ROSMUSJ\14-Jun-2012\0\#p
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\title\0,1\N\C,1,1.4602097254\H,1,1.0118942728,2,110.65031695\H,1,1.
0118949933,2,110.65398095,3,118.0749232,0\H,2,1.0951719958,1,114.8201245,4,59.01
82916,0\H,2,1.0891933689,1,109.15702172,4,-
62.49154993,0\H,2,1.0891805356,1,109.15157491,4,180.52082991,0\Version=EM64M
-G09RevC.01\State=1-A\HF=-95.2608142\RMSD=4.738e-09\Dipole=0.2650043,-
0.4416546,0.1485198\Quadrupole=0.5576828,-0.2805395,-0.2771434,0.7855983,-
0.8134837,1.3560521\PG=C01 [X(C1H5N1)]\@

```

HF=-95.8412109

```

Sum of electronic and zero-point Energies=      -95.776905
Sum of electronic and thermal Energies=         -95.773460
Sum of electronic and thermal Enthalpies=       -95.772516
Sum of electronic and thermal Free Energies=    -95.799841
NImag=0

```

C2H10B1N1

-----

```

0,1
B
N,1,r2
H,1,r3,2,a3
H,1,r4,2,a4,3,d4,0
H,1,r5,2,a5,3,d5,0
C,2,r6,1,a6,3,d6,0
C,2,r7,1,a7,3,d7,0
H,2,r8,1,a8,3,d8,0
H,6,r9,2,a9,1,d9,0
H,6,r10,2,a10,1,d10,0
H,6,r11,2,a11,1,d11,0
H,7,r12,2,a12,1,d12,0
H,7,r13,2,a13,1,d13,0

```

H,7,r14,2,a14,1,d14,0

r2=1.63223572  
r3=1.20673379  
r4=1.20672768  
r5=1.20861525  
r6=1.47309072  
r7=1.4733254  
r8=1.01677855  
r9=1.09072194  
r10=1.08612831  
r11=1.08792612  
r12=1.09058873  
r13=1.08788624  
r14=1.08615067  
a3=105.55332657  
a4=105.51846282  
a5=104.73097217  
a6=111.61734643  
a7=111.48268058  
a8=106.07708883  
a9=110.91268432  
a10=108.8515046  
a11=107.75055953  
a12=110.9841692  
a13=107.71669131  
a14=108.79125807  
d4=120.36047855  
d5=240.18756842  
d6=181.73151993  
d7=56.84141284  
d8=299.32605328  
d9=179.22388338  
d10=57.4691804  
d11=299.57663502  
d12=180.63056648  
d13=60.2467565  
d14=302.42533311

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-  
311++G(3df,2p)\C2H10B1N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\C,2,r  
6,1,a6,3,d6,0\C,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d10  
,0\H,6,r11,2,a11,1,d11,0\H,7,r12,2,a12,1,d12,0\H,7,r13,2,a13,1,d13,0\H,7,r14,2,a14,1,d1

```

4,0\r2=1.63223572\r3=1.20673379\r4=1.20672768\r5=1.20861525\r6=1.47309072\r7=1
.4733254\r8=1.01677855\r9=1.09072194\r10=1.08612831\r11=1.08792612\r12=1.09058
873\r13=1.08788624\r14=1.08615067\a3=105.55332657\a4=105.51846282\a5=104.7309
7217\a6=111.61734643\a7=111.48268058\a8=106.07708883\a9=110.91268432\a10=108
.8515046\a11=107.75055953\a12=110.9841692\a13=107.71669131\a14=108.79125807\
d4=120.36047855\d5=240.18756842\d6=181.73151993\d7=56.84141284\d8=299.32605
328\d9=179.22388338\d10=57.4691804\d11=299.57663502\d12=180.63056648\d13=60.
2467565\d14=302.42533311\\Version=EM64M-G09RevC.01\State=1-A\HF=-
135.1373343\RMSD=6.025e-09\RMSF=8.828e-05\Dipole=-
0.0323263,0.0597195,1.9954068\Quadrupole=2.0998765,1.7650645,-
3.8649409,0.2708564,0.6514146,-1.1727094\PG=C01 [X(C2H10B1N1)]\@
--- NBO Single Point ---
1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\C2H10B1N1\ROSMUSJ\18-Jun-
2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read
geom=allcheck\title\0,1\B\N,1,1.632235719\H,1,1.2067337904,2,105.55332657\H,1,1.2
067276759,2,105.51846282,3,120.36047855,0\H,1,1.208615252,2,104.73097217,3,240.1
8756842,0\C,2,1.4730907165,1,111.61734643,3,181.73151993,0\C,2,1.473325404,1,111
.48268058,3,56.84141284,0\H,2,1.0167785485,1,106.07708883,3,299.32605328,0\H,6,1.
090721944,2,110.91268432,1,179.22388338,0\H,6,1.0861283107,2,108.8515046,1,57.46
91804,0\H,6,1.0879261181,2,107.75055953,1,299.57663502,0\H,7,1.0905887303,2,110.
9841692,1,180.63056648,0\H,7,1.0878862408,2,107.71669131,1,60.2467565,0\H,7,1.08
61506743,2,108.79125807,1,302.42533311,0\\Version=EM64M-G09RevC.01\State=1-
A\HF=-160.7451258\RMSD=9.838e-09\Dipole=-
0.0320428,0.059482,2.0679588\Quadrupole=2.1564392,1.8846288,-
4.041068,0.2185973,0.6896171,-1.2414404\PG=C01 [X(C2H10B1N1)]\@

```

HF=-135.1373343

```

Sum of electronic and zero-point Energies=      -161.668614
Sum of electronic and thermal Energies=         -161.662783
Sum of electronic and thermal Enthalpies=       -161.661839
Sum of electronic and thermal Free Energies=    -161.696383
NImag=0

```

C2H7N1

```

-----
0,1
N
C,1,r2
C,1,r3,2,a3
H,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,2,r6,1,a6,4,d6,0
H,2,r7,1,a7,4,d7,0
H,3,r8,1,a8,2,d8,0

```

H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0

r2=1.45148325  
r3=1.45145317  
r4=1.01157682  
a3=112.11825435  
a4=109.7660691  
d4=122.27339611  
r5=1.09980696  
r6=1.08902956  
r7=1.0913865  
a5=113.45588839  
a6=109.97975571  
a7=109.13845553  
d5=67.8874186  
d6=-53.942204  
d7=187.9276399  
r8=1.0890225  
r9=1.09980696  
r10=1.09138161  
a8=109.9796875  
a9=113.45405506  
a10=109.13768309  
d8=176.15589654  
d9=54.32975526  
d10=-65.71192905

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\C2H7N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\C,1,r2\C,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\|r2=1.45148325\r3=1.45145317\r4=1.01157682\a3=112.11825435\a4=109.7660691\d4=122.27339611\r5=1.09980696\r6=1.08902956\r7=1.0913865\a5=113.45588839\a6=109.97975571\a7=109.13845553\d5=67.8874186\d6=-53.942204\d7=187.9276399\r8=1.0890225\r9=1.09980696\r10=1.09138161\a8=109.9796875\a9=113.45405506\a10=109.13768309\d8=176.15589654\d9=54.32975526\d10=-65.71192905\|Version=EM64M-G09RevC.01\State=1-A\HF=-135.138592\RMSD=3.080e-09\RMSF=5.843e-05\Dipole=0.1377647,-0.3700762,0.0927249\Quadrupole=-0.1947625,-0.1066657,0.3014283,1.3223863,-0.6100306,0.8902552\PG=C01 [X(C2H7N1)]\|@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\C2H7N1\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\C,1,1.4514832475\C,1,1.4514531693,2,112.11825435\H,1,1.

0115768169,2,109.7660691,3,122.27339611,0\H,2,1.0998069624,1,113.45588839,4,67.8  
874186,0\H,2,1.0890295594,1,109.97975571,4,-  
53.942204,0\H,2,1.0913864962,1,109.13845553,4,187.9276399,0\H,3,1.0890224986,1,1  
09.9796875,2,176.15589654,0\H,3,1.0998069582,1,113.45405506,2,54.32975526,0\H,3,  
1.0913816136,1,109.13768309,2,-65.71192905,0\Version=EM64M-  
G09RevC.01\State=1-A\HF=-134.30231\RMSD=5.028e-09\Dipole=0.1401968,-  
0.3815973,0.0943612\Quadrupole=-0.1831532,-0.0675582,0.2507114,1.2974792,-  
0.5333675,0.8734871\PG=C01 [X(C2H7N1)]\@

HF=-135.138592

Sum of electronic and zero-point Energies= -135.045774  
Sum of electronic and thermal Energies= -135.041351  
Sum of electronic and thermal Enthalpies= -135.040407  
Sum of electronic and thermal Free Energies= -135.071268  
NImag=0

C3H12B1N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
C,2,r6,1,a6,3,d6,0  
C,2,r7,1,a7,3,d7,0  
C,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,6,r10,2,a10,1,d10,0  
H,6,r11,2,a11,1,d11,0  
H,7,r12,2,a12,1,d12,0  
H,7,r13,2,a13,1,d13,0  
H,7,r14,2,a14,1,d14,0  
H,8,r15,2,a15,1,d15,0  
H,8,r16,2,a16,1,d16,0  
H,8,r17,2,a17,1,d17,0

r2=1.63922274  
r3=1.20732792  
r4=1.20739584  
r5=1.2072536  
r6=1.47515235  
r7=1.47528871  
r8=1.47530987

r9=1.0920814  
r10=1.08683481  
r11=1.08683652  
r12=1.09208016  
r13=1.08703978  
r14=1.086927  
r15=1.09202397  
r16=1.08707543  
r17=1.08687285  
a3=105.3247753  
a4=105.34844742  
a5=105.31310193  
a6=109.59737583  
a7=109.56857584  
a8=109.53163401  
a9=110.24497557  
a10=108.60055327  
a11=108.59430968  
a12=110.26567162  
a13=108.62511588  
a14=108.53894346  
a15=110.28115543  
a16=108.55294572  
a17=108.58001841  
d4=120.12159195  
d5=240.11616671  
d6=179.23401111  
d7=59.20423756  
d8=299.21934488  
d9=179.83161814  
d10=59.08437053  
d11=300.64006049  
d12=179.75988405  
d13=58.88386068  
d14=300.53989518  
d15=179.5614837  
d16=58.73400542  
d17=300.39139057

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\FOpt\RM062X\6-  
311++G(3df,2p)\C3H12B1N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\C,2,r  
6,1,a6,3,d6,0\C,2,r7,1,a7,3,d7,0\C,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d10  
,0\H,6,r11,2,a11,1,d11,0\H,7,r12,2,a12,1,d12,0\H,7,r13,2,a13,1,d13,0\H,7,r14,2,a14,1,d1



4,0\H,8,r15,2,a15,1,d15,0\H,8,r16,2,a16,1,d16,0\H,8,r17,2,a17,1,d17,0\r2=1.63922274\r3=1.20732792\r4=1.20739584\r5=1.2072536\r6=1.47515235\r7=1.47528871\r8=1.47530987\r9=1.0920814\r10=1.08683481\r11=1.08683652\r12=1.09208016\r13=1.08703978\r14=1.086927\r15=1.09202397\r16=1.08707543\r17=1.08687285\a3=105.3247753\a4=105.34844742\a5=105.31310193\a6=109.59737583\a7=109.56857584\a8=109.53163401\a9=110.24497557\a10=108.60055327\a11=108.59430968\a12=110.26567162\a13=108.62511588\a14=108.53894346\a15=110.28115543\a16=108.55294572\a17=108.58001841\d4=120.12159195\d5=240.11616671\d6=179.23401111\d7=59.20423756\d8=299.21934488\d9=179.83161814\d10=59.08437053\d11=300.64006049\d12=179.75988405\d13=58.88386068\d14=300.53989518\d15=179.5614837\d16=58.73400542\d17=300.39139057\Version=EM64M-G09RevC.01\State=1-A\HF=-174.4383496\RMSD=3.440e-09\RMSF=7.848e-05\Dipole=0.0004268,-0.0009306,1.9210209\Quadrupole=2.3523829,2.3568087,-4.7091916,0.0021915,-0.0036866,0.0022354\PG=C01 [X(C3H12B1N1)]\@\n\n--- NBO Single Point ---\n1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\C3H12B1N1\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read\ngeom=allcheck\title\0,1\B\N,1,1.6392227445\H,1,1.2073279236,2,105.3247753\H,1,1.2073958428,2,105.34844742,3,120.12159195,0\H,1,1.2072535978,2,105.31310193,3,240.11616671,0\C,2,1.4751523502,1,109.59737583,3,179.23401111,0\C,2,1.4752887086,1,109.56857584,3,59.20423756,0\C,2,1.4753098742,1,109.53163401,3,299.21934488,0\H,6,1.0920813981,2,110.24497557,1,179.83161814,0\H,6,1.0868348111,2,108.60055327,1,59.08437053,0\H,6,1.0868365166,2,108.59430968,1,300.64006049,0\H,7,1.0920801569,2,110.26567162,1,179.75988405,0\H,7,1.0870397763,2,108.62511588,1,58.88386068,0\H,7,1.0869270022,2,108.53894346,1,300.53989518,0\H,8,1.0920239687,2,110.28115543,1,179.5614837,0\H,8,1.0870754297,2,108.55294572,1,58.73400542,0\H,8,1.0868728482,2,108.58001841,1,300.39139057,0\Version=EM64M-G09RevC.01\State=1-A\HF=-199.7867774\RMSD=8.866e-09\Dipole=0.0004392,-0.0009901,1.9941086\Quadrupole=2.4377665,2.442038,-4.8798045,0.0018448,-0.0034858,0.0022319\PG=C01 [X(C3H12B1N1)]\@\n\n

HF=-174.4383496

Sum of electronic and zero-point Energies= -200.943237  
Sum of electronic and thermal Energies= -200.936452  
Sum of electronic and thermal Enthalpies= -200.935508  
Sum of electronic and thermal Free Energies= -200.972215  
NImag=0

C3H9N1

-----  
0,1  
N  
C,1,r2  
C,1,r3,2,a3

C,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0  
H,4,r11,1,a11,3,d11,0  
H,4,r12,1,a12,3,d12,0  
H,4,r13,1,a13,3,d13,0

r2=1.44903478  
r3=1.44901212  
r4=1.44899887  
a3=110.75779836  
a4=110.74527192  
d4=123.18274026  
r5=1.10338601  
r6=1.08994892  
r7=1.08992978  
a5=112.10391305  
a6=109.83917364  
a7=109.84934788  
d5=61.52188044  
d6=-58.92236314  
d7=181.94718604  
r8=1.0899669  
r9=1.10341426  
r10=1.08994185  
a8=109.85854891  
a9=112.12083511  
a10=109.85280715  
d8=182.24976366  
d9=61.81403032  
d10=-58.61439346  
r11=1.10338693  
r12=1.08997104  
r13=1.08993872  
a11=112.10309341  
a12=109.83998213  
a13=109.84369611  
d11=61.73315799  
d12=-58.68794587  
d13=182.18781067

--- Geometry Optimization ---

```

1\1\GINC-MH325M16MH\FOpt\RM062X\6-311++G(3df,2p)\C3H9N1\ROSMUSJ\15-
Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\N\C,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6
,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,
1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.44903478\r3=1.449012
12\r4=1.44899887\a3=110.75779836\a4=110.74527192\d4=123.18274026\r5=1.103386
01\r6=1.08994892\r7=1.08992978\a5=112.10391305\a6=109.83917364\a7=109.8493478
8\d5=61.52188044\d6=-
58.92236314\d7=181.94718604\r8=1.0899669\r9=1.10341426\r10=1.08994185\a8=109.
85854891\a9=112.12083511\a10=109.85280715\d8=182.24976366\d9=61.81403032\d1
0=-
58.61439346\r11=1.10338693\r12=1.08997104\r13=1.08993872\a11=112.10309341\a12
=109.83998213\a13=109.84369611\d11=61.73315799\d12=-
58.68794587\d13=182.18781067\Version=EM64M-G09RevC.01\State=1-A\HF=-
174.4402392\RMSD=4.286e-09\RMSF=1.135e-04\Dipole=0.1139701,-
0.2099446,0.0785622\Quadrupole=0.3516267,-0.9953421,0.6437154,1.0277511,-
0.382853,0.7111783\PG=C01 [X(C3H9N1)]\@
--- NBO Single Point ---
1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\C3H9N1\ROSMUSJ\18-Jun-2012\0\#p
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\title\0,1\N\C,1,1.4490347785\C,1,1.4490121231,2,110.75779836\C,1,1.
4489988688,2,110.74527192,3,123.18274026,0\H,2,1.103386006,1,112.10391305,4,61.5
2188044,0\H,2,1.0899489157,1,109.83917364,4,-
58.92236314,0\H,2,1.0899297777,1,109.84934788,4,181.94718604,0\H,3,1.0899668957,
1,109.85854891,2,182.24976366,0\H,3,1.1034142577,1,112.12083511,2,61.81403032,0\
H,3,1.0899418467,1,109.85280715,2,-
58.61439346,0\H,4,1.103386927,1,112.10309341,3,61.73315799,0\H,4,1.0899710415,1,
109.83998213,3,-
58.68794587,0\H,4,1.0899387231,1,109.84369611,3,182.18781067,0\Version=EM64M
-G09RevC.01\State=1-A\HF=-173.3453611\RMSD=8.256e-09\Dipole=0.12518,-
0.2309489,0.0863375\Quadrupole=0.3209775,-0.9092769,0.5882994,0.9387958,-
0.3498793,0.6496021\PG=C01 [X(C3H9N1)]\@

```

HF=-174.4402392

```

Sum of electronic and zero-point Energies=      -174.319186
Sum of electronic and thermal Energies=         -174.313823
Sum of electronic and thermal Enthalpies=       -174.312878
Sum of electronic and thermal Free Energies=     -174.346414
NImag=0

```

B1C11H5N1

```

-----
0,1
B

```

N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Cl,2,r6,1,a6,3,d6,0  
H,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0

r2=1.63590684  
r3=1.20916164  
r4=1.19953052  
r5=1.19920266  
r6=1.73306997  
r7=1.01731608  
r8=1.01694779  
a3=100.44810494  
a4=105.42538587  
a5=105.40250536  
a6=116.39669268  
a7=110.00977733  
a8=109.97449074  
d4=118.82631077  
d5=241.17502569  
d6=179.40118232  
d7=58.7633239  
d8=299.94712829

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1C11H5N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Cl,2,  
r6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\r2=1.63590684\r3=1.20916164\r4=1  
.19953052\r5=1.19920266\r6=1.73306997\r7=1.01731608\r8=1.01694779\a3=100.44810  
494\a4=105.42538587\a5=105.40250536\a6=116.39669268\a7=110.00977733\a8=109.9  
7449074\d4=118.82631077\d5=241.17502569\d6=179.40118232\d7=58.7633239\d8=29  
9.94712829\Version=EM64M-G09RevC.01\State=1-A\HF=-  
516.1089919\RMSD=5.607e-09\RMSF=1.755e-04\Dipole=0.4042243,-  
0.0039464,1.6391928\Quadrupole=2.4527772,1.3884166,-3.8411938,-  
0.0112227,2.5421821,-0.0275602\PG=C01 [X(B1C11H5N1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1C11H5N1\ROSMUSJ\14-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6359068417\H,1,1.2091616367,2,100.44810494\H,1,1.  
1995305238,2,105.42538587,3,118.82631077,0\H,1,1.199202664,2,105.40250536,3,241.  
17502569,0\Cl,2,1.73306997,1,116.39669268,3,179.40118232,0\H,2,1.017316079,1,110.

00977733,3,58.7633239,0\H,2,1.0169477867,1,109.97449074,3,299.94712829,0\Version=EM64M-G09RevC.01\State=1-A\HF=-541.5432812\RMSD=5.796e-09\Dipole=0.4177124,-0.0043645,1.7253378\Quadrupole=2.5023124,1.5110721,-4.0133845,-0.0109317,2.7588748,-0.0290383\PG=C01 [X(B1C11H5N1)]\@

HF=-516.1089919

Sum of electronic and zero-point Energies= -542.686850  
Sum of electronic and thermal Energies= -542.682462  
Sum of electronic and thermal Enthalpies= -542.681518  
Sum of electronic and thermal Free Energies= -542.713383  
NImag=0

Cl1H2N1

-----  
0,1  
N  
Cl,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.73013813  
r3=1.01574087  
r4=1.01574087  
a3=104.98426144  
a4=104.98426144  
d4=111.80333713

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\POpt\RM062X\6-311++G(3df,2p)\Cl1H2N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Cl,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.73013813\r3=1.01574087\r4=1.01574087\a3=104.98426144\a4=104.98426144\d4=111.80333713\Version=EM64M-G09RevC.01\State=1-A\HF=-516.1091964\RMSD=7.483e-09\RMSF=8.876e-05\Dipole=0.3439423,-0.5080325,-0.4627013\Quadrupole=-0.0468591,-0.6616334,0.7084925,0.768393,-1.1436132,1.6892156\PG=CS [SG(Cl1N1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\Cl1H2N1\ROSMUSJ\14-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Cl,1,1.730138129\H,1,1.0157408658,2,104.98426144\H,1,1.0157408658,2,104.98426144,3,111.80333713,0\Version=EM64M-G09RevC.01\State=1-A\HF=-515.1180817\RMSD=1.770e-09\Dipole=0.3611459,-0.5334437,-0.5110114\Quadrupole=-0.046961,-0.6412603,0.6882213,0.7428018,-1.1579216,1.7103503\PG=CS [SG(Cl1N1),X(H2)]\@

HF=-516.1091964

Sum of electronic and zero-point Energies= -516.082400  
Sum of electronic and thermal Energies= -516.079424  
Sum of electronic and thermal Enthalpies= -516.078480  
Sum of electronic and thermal Free Energies= -516.105738  
NImag=0

B1Cl2H4N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Cl,2,r6,1,a6,3,d6,0  
Cl,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0

r2=1.65051654  
r3=1.20219212  
r4=1.20226187  
r5=1.19673115  
r6=1.73417324  
r7=1.73383937  
r8=1.01987956  
a3=101.59265446  
a4=101.62914377  
a5=105.05628616  
a6=113.56677334  
a7=113.58390529  
a8=109.1098475  
d4=118.7265613  
d5=239.40200289  
d6=183.82987276  
d7=56.8582997  
d8=300.3431199

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1Cl2H4N1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Cl,2,  
r6,1,a6,3,d6,0\Cl,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\r2=1.65051654\r3=1.20219212\r4=

1.20226187\r5=1.19673115\r6=1.73417324\r7=1.73383937\r8=1.01987956\a3=101.5926  
5446\a4=101.62914377\a5=105.05628616\a6=113.56677334\a7=113.58390529\a8=109.  
1098475\d4=118.7265613\d5=239.40200289\d6=183.82987276\d7=56.8582997\d8=300.  
3431199\\Version=EM64M-G09RevC.01\State=1-A\HF=-975.6693809\RMSD=2.759e-  
09\RMSF=9.338e-05\Dipole=0.1429195,-  
0.2440078,1.402727\Quadrupole=2.1360742,2.1555227,-4.2915969,-  
0.0186004,0.5794355,-0.9876381\PG=C01 [X(B1Cl2H4N1)]\@  
--- NBO Single Point ---  
1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1Cl2H4N1\ROSMUSJ\18-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read  
geom=allcheck\\title\0,1\B\N,1,1.6505165351\H,1,1.2021921226,2,101.59265446\H,1,1.  
2022618652,2,101.62914377,3,118.7265613,0\H,1,1.1967311496,2,105.05628616,3,239.  
40200289,0\Cl,2,1.7341732385,1,113.56677334,3,183.82987276,0\Cl,2,1.7338393721,1,  
113.58390529,3,56.8582997,0\H,2,1.01987956,1,109.1098475,3,300.3431199,0\\Version  
=EM64M-G09RevC.01\State=1-A\HF=-1000.423132\RMSD=3.152e-  
09\Dipole=0.1488066,-0.2543073,1.5049446\Quadrupole=2.2366736,2.3017406,-  
4.5384143,-0.0593786,0.653896,-1.1143873\PG=C01 [X(B1Cl2H4N1)]\@

HF=-975.6693809

Sum of electronic and zero-point Energies= -1002.249431  
Sum of electronic and thermal Energies= -1002.244285  
Sum of electronic and thermal Enthalpies= -1002.243341  
Sum of electronic and thermal Free Energies= -1002.278295  
NImag=0

Cl2H1N1

-----  
0,1  
N  
Cl,1,r2  
Cl,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.73088946  
r3=1.73105085  
r4=1.01833061  
a3=110.55222775  
a4=103.54053181  
d4=110.22202979

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\Cl2H1N1\ROSMUSJ\15-  
Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\title\0,1\N\Cl,1,r2\Cl,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.73088946\r3=1.73105085\r

4=1.01833061\a3=110.55222775\a4=103.54053181\d4=110.22202979\\Version=EM64  
M-G09RevC.01\State=1-A\HF=-975.6695424\RMSD=3.637e-09\RMSF=1.754e-  
04\Dipole=-0.1645795,-0.4987176,-0.1140222\Quadrupole=0.0936578,-  
0.1453933,0.0517355,1.4446189,0.060177,1.0028221\PG=C01 [X(Cl2H1N1)]\@  
--- NBO Single Point ---  
1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\Cl2H1N1\ROSMUSJ\18-Jun-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\\title\0,1\N\Cl,1,1.7308894619\Cl,1,1.7310508532,2,110.55222775\H,1,  
1.01833061,2,103.54053181,3,110.22202979,0\\Version=EM64M-G09RevC.01\State=1-  
A\HF=-974.0088559\RMSD=3.029e-09\Dipole=-0.1822269,-0.5342439,-  
0.1262104\Quadrupole=0.0869202,-0.051802,-  
0.0351182,1.4399943,0.1674676,0.9997235\PG=C01 [X(Cl2H1N1)]\@

HF=-975.6695424

Sum of electronic and zero-point Energies=	-975.652240
Sum of electronic and thermal Energies=	-975.648711
Sum of electronic and thermal Enthalpies=	-975.647767
Sum of electronic and thermal Free Energies=	-975.678904
NImag=0	

B1Cl3H3N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Cl,2,r6,1,a6,3,d6,0  
Cl,2,r7,1,a7,3,d7,0  
Cl,2,r8,1,a8,3,d8,0

r2=1.69588734  
r3=1.19746803  
r4=1.19751549  
r5=1.19760681  
r6=1.74029655  
r7=1.74140117  
r8=1.74009613  
a3=101.60696092  
a4=101.60020969  
a5=101.59748983  
a6=110.69234705  
a7=110.60833518



a8=110.75289031  
d4=120.06096049  
d5=240.04731396  
d6=179.91831652  
d7=59.95200694  
d8=299.96944812

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1Cl3H3N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Cl,2,  
r6,1,a6,3,d6,0\Cl,2,r7,1,a7,3,d7,0\Cl,2,r8,1,a8,3,d8,0\r2=1.69588734\r3=1.19746803\r4=  
1.19751549\r5=1.19760681\r6=1.74029655\r7=1.74140117\r8=1.74009613\a3=101.6069  
6092\a4=101.60020969\a5=101.59748983\a6=110.69234705\a7=110.60833518\a8=110.  
75289031\d4=120.06096049\d5=240.04731396\d6=179.91831652\d7=59.95200694\d8=  
299.96944812\Version=EM64M-G09RevC.01\State=1-A\HF=-  
1435.2266401\RMSD=4.628e-09\RMSF=9.974e-05\Dipole=-0.0001918,-  
0.0000757,1.2557388\Quadrupole=2.2755945,2.2740984,-4.5496929,-0.0035437,-  
0.002051,-0.0091913\PG=C01 [X(B1Cl3H3N1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\B1Cl3H3N1\ROSMUSJ\18-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6958873439\H,1,1.1974680272,2,101.60696092\H,1,1.  
1975154882,2,101.60020969,3,120.06096049,0\H,1,1.1976068051,2,101.59748983,3,24  
0.04731396,0\Cl,2,1.7402965468,1,110.69234705,3,179.91831652,0\Cl,2,1.7414011659,  
1,110.60833518,3,59.95200694,0\Cl,2,1.7400961252,1,110.75289031,3,299.96944812,0  
\Version=EM64M-G09RevC.01\State=1-A\HF=-1459.2962923\RMSD=6.450e-  
09\Dipole=0.0000653,-0.00001,1.3534014\Quadrupole=2.3866494,2.385211,-  
4.7718605,0.0008693,-0.0013902,-0.0073837\PG=C01 [X(B1Cl3H3N1)]\@

HF=-1435.2266401

Sum of electronic and zero-point Energies=	-1461.808352
Sum of electronic and thermal Energies=	-1461.802146
Sum of electronic and thermal Enthalpies=	-1461.801202
Sum of electronic and thermal Free Energies=	-1461.838999
NImag=0	

Cl3N1

-----

0,1  
N  
Cl,1,r2  
Cl,1,r3,2,a3

Cl,1,r4,2,a4,3,d4,0

r2=1.73719437  
r3=1.73777094  
r4=1.73777094  
a3=108.40585018  
a4=108.40585018  
d4=117.58092661

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\POpt\RM062X\6-311++G(3df,2p)\Cl3N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Cl,1,r2\Cl,1,r3,2,a3\Cl,1,r4,2,a4,3,d4,0\r2=1.73719437\r3=1.73777094\  
r4=1.73777094\a3=108.40585018\a4=108.40585018\d4=117.58092661\Version=EM64  
M-G09RevC.01\State=1-A\HF=-1435.226626\RMSD=2.235e-09\RMSF=2.065e-  
04\Dipole=0.0787641,-0.1300061,0.0565934\Quadrupole=0.2376648,-  
0.75063,0.5129652,0.9459837,-0.4126184,0.6810581\PG=CS [SG(Cl1N1),X(Cl2)]\@

--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\Cl3N1\ROSMUSJ\18-Jun-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Cl,1,1.737194366\Cl,1,1.7377709449,2,108.40585018\Cl,1,1,  
.7377709449,2,108.40585018,3,117.58092661,0\Version=EM64M-  
G09RevC.01\State=1-A\HF=-1432.8923621\RMSD=3.383e-09\Dipole=0.0901349,-  
0.1487745,0.0652701\Quadrupole=0.2195486,-0.6862883,0.4667397,0.867056,-  
0.3775433,0.6231639\PG=CS [SG(Cl1N1),X(Cl2)]\@

HF=-1435.226626

Sum of electronic and zero-point Energies=	-1435.219880
Sum of electronic and thermal Energies=	-1435.215423
Sum of electronic and thermal Enthalpies=	-1435.214478
Sum of electronic and thermal Free Energies=	-1435.248953

NImag=0

B1F1H5N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
F,2,r6,1,a6,3,d6,0  
H,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0

r2=1.60555753  
r3=1.21219138  
r4=1.19806685  
r5=1.19843379  
r6=1.38479855  
r7=1.01936974  
r8=1.01954746  
a3=99.33678176  
a4=105.91851696  
a5=105.84078783  
a6=115.00160984  
a7=111.90302193  
a8=111.95063918  
d4=118.24854785  
d5=242.18407076  
d6=178.89235334  
d7=60.29460124  
d8=297.58273641

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1F1H5N1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\F,2,r  
6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\r2=1.60555753\r3=1.21219138\r4=1.  
19806685\r5=1.19843379\r6=1.38479855\r7=1.01936974\r8=1.01954746\a3=99.336781  
76\a4=105.91851696\a5=105.84078783\a6=115.00160984\a7=111.90302193\a8=111.95  
063918\d4=118.24854785\d5=242.18407076\d6=178.89235334\d7=60.29460124\d8=29  
7.58273641\Version=EM64M-G09RevC.01\State=1-A\HF=-  
155.7145515\RMSD=8.504e-09\RMSF=1.561e-04\Dipole=0.6783002,-  
0.0131009,1.5457113\Quadrupole=0.4697776,1.4331204,-  
1.902898,0.0183064,2.434373,-0.0504603\PG=C01 [X(B1F1H5N1)]\@\

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1F1H5N1\ROSMUSJ\14-Jun-  
2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.605557535\H,1,1.212191379,2,99.33678176\H,1,1.198  
0668508,2,105.91851696,3,118.24854785,0\H,1,1.1984337894,2,105.84078783,3,242.18  
407076,0\F,2,1.3847985548,1,115.00160984,3,178.89235334,0\H,2,1.0193697369,1,111  
.90302193,3,60.29460124,0\H,2,1.0195474582,1,111.95063918,3,297.58273641,0\Versi  
on=EM64M-G09RevC.01\State=1-A\HF=-181.4672579\RMSD=3.360e-  
09\Dipole=0.722422,-0.0149515,1.6314698\Quadrupole=0.4344857,1.579646,-  
2.0141317,0.020412,2.6817017,-0.0522459\PG=C01 [X(B1F1H5N1)]\@\

HF=-155.7145515

Sum of electronic and zero-point Energies= -182.295213  
 Sum of electronic and thermal Energies= -182.291084  
 Sum of electronic and thermal Enthalpies= -182.290140  
 Sum of electronic and thermal Free Energies= -182.320598  
 NImag=0

F1H2N1

-----  
 0,1  
 N  
 F,1,r2  
 H,1,r3,2,a3  
 H,1,r4,2,a4,3,d4,0  
 r2=1.40081468  
 r3=1.01885979  
 r4=1.01885979  
 a3=102.36270142  
 a4=102.36270142  
 d4=109.22388075

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\POpt\RM062X\6-311++G(3df,2p)\F1H2N1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
 freq\title\0,1\N\F,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.40081468\r3=1.01885979\r4=1.01885979\ a3=102.36270142\ a4=102.36270142\ d4=109.22388075\Version=EM64M-G09RevC.01\State=1-A\HF=-155.7151084\RMSD=7.493e-09\RMSF=9.056e-05\Dipole=0.4033985,-0.5678874,-0.5575322\Quadrupole=0.4368632,-0.080969,-0.3558942,0.7425092,-0.8027073,1.1300176\PG=CS [SG(F1N1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\F1H2N1\ROSMUSJ\14-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
 geom=allcheck\title\0,1\N\F,1,1.4008146815\H,1,1.0188597862,2,102.36270142\H,1,1.0188597862,2,102.36270142,3,109.22388075,0\Version=EM64M-G09RevC.01\State=1-A\HF=-155.0380799\RMSD=3.162e-09\Dipole=0.4201802,-0.5915119,-0.6465983\Quadrupole=0.4655513,-0.042461,-0.4230903,0.7284285,-0.8099828,1.1402596\PG=CS [SG(F1N1),X(H2)]\@

HF=-155.7151084

Sum of electronic and zero-point Energies= -155.687003  
 Sum of electronic and thermal Energies= -155.684114  
 Sum of electronic and thermal Enthalpies= -155.683170  
 Sum of electronic and thermal Free Energies= -155.709202  
 NImag=0

B1F2H4N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
F,2,r6,1,a6,3,d6,0  
F,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0

r2=1.60055117  
r3=1.20139032  
r4=1.20146336  
r5=1.19391962  
r6=1.35713629  
r7=1.3567224  
r8=1.02482274  
a3=101.08597013  
a4=101.01038684  
a5=105.0625984  
a6=114.47804268  
a7=114.547792  
a8=114.35039352  
d4=117.15893219  
d5=238.4897742  
d6=182.62699282  
d7=62.7367655  
d8=302.60280691

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1F2H4N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\F,2,r  
6,1,a6,3,d6,0\F,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\r2=1.60055117\r3=1.20139032\r4=1.  
20146336\r5=1.19391962\r6=1.35713629\r7=1.3567224\r8=1.02482274\a3=101.085970  
13\a4=101.01038684\a5=105.0625984\a6=114.47804268\a7=114.547792\a8=114.35039  
352\d4=117.15893219\d5=238.4897742\d6=182.62699282\d7=62.7367655\d8=302.6028  
0691\Version=EM64M-G09RevC.01\State=1-A\HF=-254.8983474\RMSD=7.382e-  
09\RMSF=1.428e-04\Dipole=0.3374131,-  
0.5258722,1.1576975\Quadrupole=0.444318,1.4151997,-1.8595177,-  
1.0508022,0.8891154,-1.3810659\PG=C01 [X(B1F2H4N1)]\@\nbo  
--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1F2H4N1\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
 geom=allcheck\title\0,1\B\N,1,1.6005511685\H,1,1.2013903214,2,101.08597013\H,1,1.2014633597,2,101.01038684,3,117.15893219,0\H,1,1.1939196213,2,105.0625984,3,238.4897742,0\F,2,1.357136294,1,114.47804268,3,182.62699282,0\F,2,1.3567223979,1,114.547792,3,62.7367655,0\H,2,1.0248227395,1,114.35039352,3,302.60280691,0\Version=EM64M-G09RevC.01\State=1-A\HF=-280.2860509\RMSD=3.843e-09\Dipole=0.363545,-0.5657964,1.2440204\Quadrupole=0.4410429,1.5328915,-1.9739344,-1.182267,0.9867839,-1.5355527\PG=C01 [X(B1F2H4N1)]\@

HF=-254.8983474

Sum of electronic and zero-point Energies= -281.478001  
 Sum of electronic and thermal Energies= -281.473436  
 Sum of electronic and thermal Enthalpies= -281.472492  
 Sum of electronic and thermal Free Energies= -281.504887  
 NImag=0

F2H1N1

-----  
 0,1  
 N  
 F,1,r2  
 F,1,r3,2,a3  
 H,1,r4,2,a4,3,d4,0

r2=1.37271946  
 r3=1.37272753  
 r4=1.02523949  
 a3=103.21249582  
 a4=100.95423681  
 d4=104.13795641

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\F2H1N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
 freq\title\0,1\N\F,1,r2\F,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.37271946\r3=1.37272753\r4=1.02523949\a3=103.21249582\a4=100.95423681\d4=104.13795641\Version=EM64M-G09RevC.01\State=1-A\HF=-254.8993955\RMSD=7.011e-09\RMSF=2.242e-05\Dipole=-0.3306912,-0.6319675,-0.2620287\Quadrupole=-0.2851487,0.8578756,-0.5727269,1.0592868,0.6124464,0.8393882\PG=C01 [X(F2H1N1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\F2H1N1\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
 geom=allcheck\title\0,1\N\F,1,1.37271946\F,1,1.37272753,2,103.21249582\H,1,1.0252

394901,2,100.95423681,3,104.13795641,0\\Version=EM64M-G09RevC.01\\State=1-A\\HF=-253.8687675\\RMSD=3.422e-09\\Dipole=-0.3913542,-0.6617879,-0.310097\\Quadrupole=-0.3205332,1.0006168,-0.6800836,1.0732354,0.7657293,0.8504414\\PG=C01 [X(F2H1N1)]\\@

HF=-254.8993955

Sum of electronic and zero-point Energies= -254.879116  
Sum of electronic and thermal Energies= -254.876014  
Sum of electronic and thermal Enthalpies= -254.875070  
Sum of electronic and thermal Free Energies= -254.903621  
NImag=0

B1F3H3N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
F,2,r6,1,a6,3,d6,0  
F,2,r7,1,a7,3,d7,0  
F,2,r8,1,a8,3,d8,0

r2=1.64054643  
r3=1.19459442  
r4=1.19461229  
r5=1.19424538  
r6=1.33676311  
r7=1.33662648  
r8=1.33694368  
a3=100.73124002  
a4=100.85852232  
a5=100.93970838  
a6=114.91359004  
a7=114.759196  
a8=114.679706  
d4=119.88160207  
d5=239.95177551  
d6=180.54502112  
d7=60.48787265  
d8=300.65125655

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\B1F3H3N1\ROSMUS\27-Jan-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100 freq counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\F,2,r6,1,a6,3,d6,0\F,2,r7,1,a7,3,d7,0\F,2,r8,1,a8,3,d8,0\r2=1.64054643\r3=1.19459442\r4=1.19461229\r5=1.19424538\r6=1.33676311\r7=1.33662648\r8=1.33694368\a3=100.73124002\a4=100.85852232\a5=100.93970838\a6=114.91359004\a7=114.759196\a8=114.679706\d4=119.88160207\d5=239.95177551\d6=180.54502112\d7=60.48787265\d8=300.65125655\Version=IA64L-G09RevA.02\State=1-A\HF=-354.0948373\RMSD=4.589e-09\RMSF=1.404e-04\Dipole=-0.0010611,0.0006876,0.8242309\Quadrupole=0.7384373,0.7404823,-1.4789197,-0.0004626,-0.0021089,-0.001922\PG=C01 [X(B1F3H3N1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1F3H3N1\ROSMUSJ\26-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos)\title\0,1\B\N,1,1.64054643\H,1,1.19459442,2,100.73124002\H,1,1.19461229,2,100.85852232,3,119.88160207,0\H,1,1.19424538,2,100.93970838,3,239.95177551,0\F,2,1.33676311,1,114.91359004,3,180.54502112,0\F,2,1.33662648,1,114.759196,3,60.48787265,0\F,2,1.33694368,1,114.679706,3,300.65125655,0\Version=EM64M-G09RevC.01\State=1-A\HF=-379.1115338\RMSD=9.077e-09\Dipole=-0.0011755,0.0006584,0.8771284\Quadrupole=0.7516451,0.75179,-1.503435,-0.0010668,-0.0020794,-0.0013302\PG=C01 [X(B1F3H3N1)]\@

HF=-354.0948373

Sum of electronic and zero-point Energies=	-380.667527
Sum of electronic and thermal Energies=	-380.662417
Sum of electronic and thermal Enthalpies=	-380.661473
Sum of electronic and thermal Free Energies=	-380.695528
NImag=0	

F3N1

-----

0,1  
N  
F,1,r2  
F,1,r3,2,a3  
F,1,r4,2,a4,3,d4,0

r2=1.35064243  
r3=1.35090301  
r4=1.35090301  
a3=102.06224341  
a4=102.06224341  
d4=105.35656213



--- Geometry Optimization ---

```
1\1\GINC-MH325M16MH\POpt\RM062X\6-311++G(3df,2p)\F3N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\F,1,r2\F,1,r3,2,a3\F,1,r4,2,a4,3,d4,0\r2=1.35064243\r3=1.35090301\r4=  
1.35090301\a3=102.06224341\a4=102.06224341\d4=105.35656213\Version=EM64M-  
G09RevC.01\State=1-A\HF=-354.0958907\RMSD=8.715e-09\RMSF=1.089e-  
04\Dipole=-0.0450271,0.0590601,-0.0358589\Quadrupole=-0.0001811,-  
0.0009477,0.0011287,0.0013957,-0.001885,0.0024725\PG=CS [SG(F1N1),X(F2)]\@
```

--- NBO Single Point ---

```
1\1\GINC-MH325M13MH\Freq\RHF\CC-pVQZ\F3N1\ROSMUSJ\19-Jun-2012\1\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos)  
freq\title\0,1\N\F,1,r2\F,1,r3,2,a3\F,1,r4,2,a4,3,d4,0\r2=1.35064242\r3=1.35090301\r4=  
1.35090301\a3=102.06224522\a4=102.06224522\d4=105.35656512\Version=EM64M-  
G09RevC.01\State=1-A\HF=-352.7096335\RMSD=8.726e-09\RMSF=2.026e-  
02\ZeroPoint=0.0118413\Thermal=0.0152009\Dipole=-0.0703637,0.0922929,-  
0.0566423\DipoleDeriv=1.274759,0.2991139,-  
0.184221,0.2991139,1.1104674,0.2416346,-0.1843076,0.2417482,1.3529809,-  
0.1724317,-0.0143291,-0.0774711,-0.0143291,-0.1645613,0.1016155,0.1629574,-  
0.2137441,-0.9087008,-0.8593926,-0.2118426,0.3097425,0.096356,-0.1647241,-  
0.0352353,0.0692675,0.0306685,-0.22214,-0.2429346,-0.0729422,-0.0480504,-  
0.3811407,-0.7811821,-0.3080148,-0.0479173,-0.0586726,-  
0.22214\Polar=15.1570674,2.24476,13.9241084,-  
1.3820228,1.8127384,15.7399797\PolarDeriv=-  
8.0320487,0.7661269,0.8799499,1.507692,0.5875128,-  
0.978041,1.5356967,1.4666661,7.8453964,0.5875128,1.1849942,1.2828533,1.0306984,0  
.5866655,0.708466,-0.3917006,0.5137765,-8.3111159,-  
0.5698736,0.3911609,0.0625686,2.1540051,-0.014047,0.0485267,-0.0695622,-  
0.2886844,0.7349718,-0.014047,2.1617205,-0.0636503,0.6005736,0.161404,0.5119206,-  
1.038188,1.3617455,11.7285274,10.7790524,1.3505025,0.5142005,-2.7698907,-  
0.0434379,1.1814522,-0.0689545,2.0557579,0.7358774,-0.0142488,-0.7343152,-  
0.0631968,-1.3801224,-0.2190096,-0.045707,2.4745428,0.4037482,-1.7087057,-  
2.1771301,-2.5077903,-1.456719,-0.8918064,-0.530028,-0.2519378,-1.3971799,-  
3.2337396,-9.3162456,-0.5592171,-2.6123995,-1.1560062,-0.2511496,-0.5290599,-  
1.1746797,-1.0446542,-2.2792702,-1.7087057\HyperPolar=-4.4077624,2.3255881,-  
2.1012817,6.2120383,-0.7197469,1.7902733,-1.7030741,-1.1894065,1.5600921,-  
3.8122894\PG=CS [SG(F1N1),X(F2)]\NImag=0\0.46648484,-  
0.03253360,0.48435428,0.02010285,-0.02636803,0.45843220,-0.09017471,0.00314026,-  
0.04639881,0.09439410,0.00314026,-0.09189953,0.06085928,0.01124996,0.08821493,-  
0.02009549,0.02635837,-0.28802653,-0.01929148,0.02530379,0.36400045,-  
0.29243870,0.02651212,0.02313500,-0.00976372,-  
0.00316695,0.05129464,0.34367675,0.06016015,-0.09194374,-0.00963157,-  
0.00701921,0.00949632,-0.00173852,0.02691333,0.08813390,-0.00319164,-  
0.00242565,-0.08520283,0.08080682,-0.00651579,-0.03798696,-  
0.07261395,0.00568504,0.11406208,-0.08387144,0.00288123,0.00316096,0.00554433,-  
0.01122327,-0.01190766,-0.04147433,-0.08005427,-0.00500124,0.11980144,-  
0.03076681,-0.30051100,-0.02485968,-0.00737101,-0.00581172,-0.04992364,-
```

0.05025850,-0.00568648,0.00325640,0.08839631,0.31200921,0.00318427,0.00243531,-  
0.08520283,-0.01511653,-0.07964728,-0.03798696,-  
0.00181569,0.00568505,0.00912771,0.01374794,0.07152692,0.11406208\\-  
0.02392251,0.03137810,-0.01933093,0.00053142,-0.00069704,0.03145100,0.03106554,-  
0.00057294,-0.00606004,-0.00767445,-0.03010812,-0.00606004\\\\@

HF=-352.7096335

Sum of electronic and zero-point Energies= -352.697792  
Sum of electronic and thermal Energies= -352.694433  
Sum of electronic and thermal Enthalpies= -352.693488  
Sum of electronic and thermal Free Energies= -352.723781  
NImag=0

B1Ge1H8N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Ge,2,r6,1,a6,3,d6,0  
H,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,6,r10,2,a10,1,d10,0  
H,6,r11,2,a11,1,d11,0

r2=1.65010827  
r3=1.20364152  
r4=1.20624321  
r5=1.2108889  
r6=1.90861105  
r7=1.01582245  
r8=1.01531489  
r9=1.54366207  
r10=1.52861889  
r11=1.53133516  
a3=106.93796891  
a4=104.97877331  
a5=104.84199247  
a6=108.17960993  
a7=109.11478758  
a8=109.41904449

a9=107.25884024  
a10=106.29781452  
a11=105.36621066  
d4=121.04175256  
d5=239.55911136  
d6=168.43138455  
d7=47.56634088  
d8=291.56520415  
d9=166.41223095  
d10=46.65642665  
d11=284.95575126

--- Geometry Optimization ---

```
1\1\GINC-MH325M14MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1Ge1H8N1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p)  
opt=(calcfz,z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Ge,2  
,r6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d  
10,0\H,6,r11,2,a11,1,d11,0\r2=1.65010827\r3=1.20364152\r4=1.20624321\r5=1.210888  
9\r6=1.90861105\r7=1.01582245\r8=1.01531489\r9=1.54366207\r10=1.52861889\r11=1  
.53133516\A3=106.93796891\A4=104.97877331\A5=104.84199247\A6=108.17960993\A7  
=109.11478758\A8=109.41904449\A9=107.25884024\A10=106.29781452\A11=105.36621  
066\d4=121.04175256\d5=239.55911136\d6=168.43138455\d7=47.56634088\d8=291.56  
520415\d9=166.41223095\d10=46.65642665\d11=284.95575126\Version=EM64M-  
G09RevC.01\State=1-A\HF=-2134.7200585\RMSD=2.974e-09\RMSF=3.338e-  
05\Dipole=-0.2774076,0.0608797,1.9344086\Quadrupole=2.9085902,2.3840901,-  
5.2926803,-0.1006003,4.5537434,-0.8465544\PG=C01 [X(B1Ge1H8N1)]\@\
```

--- NBO Single Point ---

```
1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1Ge1H8N1\ROSMUSJ\14-Jun-  
2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.650108265\H,1,1.2036415188,2,106.93796891\H,1,1.  
2062432107,2,104.97877331,3,121.04175256,0\H,1,1.2108889017,2,104.84199247,3,23  
9.55911136,0\Ge,2,1.9086110487,1,108.17960993,3,168.43138455,0\H,2,1.0158224505,  
1,109.11478758,3,47.56634088,0\H,2,1.0153148908,1,109.41904449,3,291.56520415,0\  
H,6,1.5436620741,2,107.25884024,1,166.41223095,0\H,6,1.5286188858,2,106.2978145  
2,1,46.65642665,0\H,6,1.5313351607,2,105.36621066,1,284.95575126,0\Version=EM6  
4M-G09RevC.01\State=1-A\HF=-2159.2301539\RMSD=5.718e-09\Dipole=-  
0.2749139,0.0585566,1.9986669\Quadrupole=2.9758536,2.4884598,-5.4643135,-  
0.0967005,4.7678856,-0.8887654\PG=C01 [X(B1Ge1H8N1)]\@\
```

HF=-2134.7200585

Sum of electronic and zero-point Energies=	-2161.284955
Sum of electronic and thermal Energies=	-2161.279196
Sum of electronic and thermal Enthalpies=	-2161.278252
Sum of electronic and thermal Free Energies=	-2161.313792

NImag=0

Ge1H5N1

0,1

N

Ge,1,r2

H,1,r3,2,a3

H,1,r4,2,a4,3,d4,0

H,2,r5,1,a5,4,d5,0

H,2,r6,1,a6,4,d6,0

H,2,r7,1,a7,4,d7,0

r2=1.84611355

r3=1.01045044

r4=1.01045441

a3=115.51615474

a4=115.42160732

d4=127.71555447

r5=1.5503057

r6=1.54062944

r7=1.54067526

a5=113.95346138

a6=106.91525574

a7=107.00145768

d5=64.92249787

d6=-55.44231777

d7=185.30204411

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\Ge1H5N1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Ge,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.84611355\r3=1.01045044\r4=1.01045441\a3=115.51615474\n4=115.42160732\d4=127.71555447\r5=1.5503057\r6=1.54062944\r7=1.54067526\a5=113.95346138\a6=106.91525574\a7=107.00145768\d5=64.92249787\d6=-55.44231777\d7=185.30204411\Version=EM64M-G09RevC.01\State=1-A\HF=-2134.7226902\RMSD=1.505e-09\RMSF=6.679e-05\Dipole=0.1725681,-0.3515586,-0.0825694\Quadrupole=0.4870691,-0.842382,0.355313,0.8637551,-0.9356548,1.8871727\PG=C01 [X(Ge1H5N1)]\@\

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\Ge1H5N1\ROSMUSJ\14-Jun-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Ge,1,1.846113549\H,1,1.0104504404,2,115.51615474\H,1,1.0104544054,2,115.42160732,3,127.71555447,0\H,2,1.5503057005,1,113.95346138,4,64.

92249787,0\H,2,1.5406294386,1,106.91525574,4,-  
55.44231777,0\H,2,1.5406752603,1,107.00145768,4,185.30204411,0\Version=EM64M  
-G09RevC.01\State=1-A\HF=-2132.7984279\RMSD=9.232e-09\Dipole=0.1833581,-  
0.3734363,-0.0936384\Quadrupole=0.4736061,-0.8169622,0.3433561,0.8383652,-  
0.9513691,1.9195239\PG=C01 [X(Ge1H5N1)]\@

HF=-2134.7226902

Sum of electronic and zero-point Energies= -2134.673750  
Sum of electronic and thermal Energies= -2134.669471  
Sum of electronic and thermal Enthalpies= -2134.668527  
Sum of electronic and thermal Free Energies= -2134.699767  
NImag=0

B1Ge2H10N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Ge,2,r6,1,a6,3,d6,0  
Ge,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,6,r10,2,a10,1,d10,0  
H,6,r11,2,a11,1,d11,0  
H,7,r12,2,a12,1,d12,0  
H,7,r13,2,a13,1,d13,0  
H,7,r14,2,a14,1,d14,0

r2=1.65508704  
r3=1.21009946  
r4=1.20484199  
r5=1.21262395  
r6=1.90126096  
r7=1.90291559  
r8=1.01668899  
r9=1.54503214  
r10=1.53047754  
r11=1.53567517  
r12=1.54718472  
r13=1.53078556  
r14=1.53264643

a3=106.90754387  
a4=106.7416689  
a5=104.76551702  
a6=106.77051893  
a7=106.47764205  
a8=107.9673993  
a9=107.22570774  
a10=107.75379531  
a11=104.92366676  
a12=107.05088565  
a13=105.95337034  
a14=106.90405588  
d4=121.68120127  
d5=241.2536678  
d6=163.65117858  
d7=38.5921843  
d8=281.83733014  
d9=163.03998611  
d10=42.61046545  
d11=280.77337293  
d12=167.87227599  
d13=49.15084529  
d14=286.8769848

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1Ge2H10N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Ge,2  
,r6,1,a6,3,d6,0\Ge,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,  
d10,0\H,6,r11,2,a11,1,d11,0\H,7,r12,2,a12,1,d12,0\H,7,r13,2,a13,1,d13,0\H,7,r14,2,a14,1  
,d14,0\r2=1.65508704\r3=1.21009946\r4=1.20484199\r5=1.21262395\r6=1.90126096\r  
7=1.90291559\r8=1.01668899\r9=1.54503214\r10=1.53047754\r11=1.53567517\r12=1.5  
4718472\r13=1.53078556\r14=1.53264643\ a3=106.90754387\ a4=106.7416689\ a5=104.7  
6551702\ a6=106.77051893\ a7=106.47764205\ a8=107.9673993\ a9=107.22570774\ a10=1  
07.75379531\ a11=104.92366676\ a12=107.05088565\ a13=105.95337034\ a14=106.90405  
588\ d4=121.68120127\ d5=241.2536678\ d6=163.65117858\ d7=38.5921843\ d8=281.8373  
3014\ d9=163.03998611\ d10=42.61046545\ d11=280.77337293\ d12=167.87227599\ d13=  
49.15084529\ d14=286.8769848\ Version=EM64M-G09RevC.01\ State=1-A\ HF=-  
4212.8941698\ RMSD=5.094e-09\ RMSF=7.846e-05\ Dipole=-  
0.0223331,0.1431408,1.7242238\ Quadrupole=4.6304498,2.2901505,-  
6.9206004,0.4568718,0.5205694,-2.5151963\ PG=C01 [X(B1Ge2H10N1)]\ \@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1Ge2H10N1\ROSMUSJ\18-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6550870419\H,1,1.2100994628,2,106.90754387\H,1,1.

2048419896,2,106.7416689,3,121.68120127,0\H,1,1.2126239476,2,104.76551702,3,241.2536678,0\Ge,2,1.9012609619,1,106.77051893,3,163.65117858,0\Ge,2,1.9029155926,1,106.47764205,3,38.5921843,0\H,2,1.016688985,1,107.9673993,3,281.83733014,0\H,6,1.545032137,2,107.22570774,1,163.03998611,0\H,6,1.5304775432,2,107.75379531,1,42.61046545,0\H,6,1.5356751667,2,104.92366676,1,280.77337293,0\H,7,1.5471847217,2,107.05088565,1,167.87227599,0\H,7,1.5307855649,2,105.95337034,1,49.15084529,0\H,7,1.5326464271,2,106.90405588,1,286.8769848,0\Version=EM64M-G09RevC.01\State=1-A\HF=-4235.8015339\RMSD=5.613e-09\Dipole=-0.0224593,0.1382766,1.792747\Quadrupole=4.6467845,2.46226,-7.1090445,0.4278089,0.5545294,-2.6594971\PG=C01 [X(B1Ge2H10N1)]\@

HF=-4212.8941698

Sum of electronic and zero-point Energies= -4239.447731  
 Sum of electronic and thermal Energies= -4239.439645  
 Sum of electronic and thermal Enthalpies= -4239.438700  
 Sum of electronic and thermal Free Energies= -4239.480937  
 NImag=0

Ge2H7N1

-----  
 0,1  
 N  
 Ge,1,r2  
 Ge,1,r3,2,a3  
 H,1,r4,2,a4,3,d4,0  
 H,2,r5,1,a5,4,d5,0  
 H,2,r6,1,a6,4,d6,0  
 H,2,r7,1,a7,4,d7,0  
 H,3,r8,1,a8,2,d8,0  
 H,3,r9,1,a9,2,d9,0  
 H,3,r10,1,a10,2,d10,0

r2=1.83697064  
 r3=1.8370824  
 r4=1.00945501  
 a3=128.33815984  
 a4=115.87368817  
 d4=179.89909983  
 r5=1.54627202  
 r6=1.54623708  
 r7=1.54095565  
 a5=110.80802925  
 a6=110.76390912  
 a7=106.45090848

d5=60.27341432  
d6=-60.00642793  
d7=180.13997408  
r8=1.54623013  
r9=1.54629253  
r10=1.54097817  
a8=110.74436904  
a9=110.81771068  
a10=106.46432719  
d8=239.72229504  
d9=119.45146916  
d10=-0.42315851

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\Ge2H7N1\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Ge,1,r2\Ge,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,  
d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=1  
.83697064\r3=1.8370824\r4=1.00945501\a3=128.33815984\a4=115.87368817\d4=179.8  
9909983\r5=1.54627202\r6=1.54623708\r7=1.54095565\a5=110.80802925\a6=110.7639  
0912\a7=106.45090848\d5=60.27341432\d6=-  
60.00642793\d7=180.13997408\r8=1.54623013\r9=1.54629253\r10=1.54097817\a8=110  
.74436904\a9=110.81771068\a10=106.46432719\d8=239.72229504\d9=119.45146916\d  
10=-0.42315851\Version=EM64M-G09RevC.01\State=1-A\HF=-  
4212.8993567\RMSD=2.751e-09\RMSF=7.822e-05\Dipole=-0.1728994,-0.0006071,-  
0.0838664\Quadrupole=1.3019426,-  
1.4478619,0.1459194,0.0064831,0.7328113,0.0020913\PG=C01 [X(Ge2H7N1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\Ge2H7N1\ROSMUSJ\18-Jun-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Ge,1,1.8369706373\Ge,1,1.8370823963,2,128.33815984\H,1  
,1.009455009,2,115.87368817,3,179.89909983,0\H,2,1.54627202,1,110.80802925,4,60.2  
7341432,0\H,2,1.5462370759,1,110.76390912,4,-  
60.00642793,0\H,2,1.5409556456,1,106.45090848,4,180.13997408,0\H,3,1.5462301319,  
1,110.74436904,2,239.72229504,0\H,3,1.5462925317,1,110.81771068,2,119.45146916,0  
\H,3,1.5409781696,1,106.46432719,2,-0.42315851,0\Version=EM64M-  
G09RevC.01\State=1-A\HF=-4209.3764823\RMSD=5.066e-09\Dipole=-0.1869334,-  
0.0007369,-0.090662\Quadrupole=1.3288875,-  
1.3576249,0.0287374,0.0065273,0.8240376,0.0022487\PG=C01 [X(Ge2H7N1)]\@

HF=-4212.8993567

Sum of electronic and zero-point Energies=	-4212.837021
Sum of electronic and thermal Energies=	-4212.830060
Sum of electronic and thermal Enthalpies=	-4212.829116
Sum of electronic and thermal Free Energies=	-4212.870044



NImag=0

B1Ge3H12N1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Ge,2,r6,1,a6,3,d6,0  
Ge,2,r7,1,a7,3,d7,0  
Ge,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,6,r10,2,a10,1,d10,0  
H,6,r11,2,a11,1,d11,0  
H,7,r12,2,a12,1,d12,0  
H,7,r13,2,a13,1,d13,0  
H,7,r14,2,a14,1,d14,0  
H,8,r15,2,a15,1,d15,0  
H,8,r16,2,a16,1,d16,0  
H,8,r17,2,a17,1,d17,0

r2=1.66135823  
r3=1.21118342  
r4=1.21139556  
r5=1.21070704  
r6=1.901097  
r7=1.90099814  
r8=1.90099107  
r9=1.54748494  
r10=1.53220434  
r11=1.53720193  
r12=1.54749145  
r13=1.53251098  
r14=1.53724621  
r15=1.54765752  
r16=1.53241957  
r17=1.53726137  
a3=106.52693204  
a4=106.47354729  
a5=106.61709918  
a6=105.27772747  
a7=105.35589266  
a8=105.3981512

a9=106.97975608  
a10=107.545671  
a11=106.20109743  
a12=106.89856324  
a13=107.45393523  
a14=106.28305898  
a15=106.90167218  
a16=107.55619342  
a17=106.16359733  
d4=119.66545875  
d5=239.65375217  
d6=161.40369624  
d7=41.40067475  
d8=281.35720565  
d9=164.96571991  
d10=45.34301476  
d11=283.09896109  
d12=165.1194615  
d13=45.51093008  
d14=283.3382942  
d15=164.68703757  
d16=45.1498143  
d17=282.8302991

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1Ge3H12N1\ROSMUSJ\17-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Ge,2  
,r6,1,a6,3,d6,0\Ge,2,r7,1,a7,3,d7,0\Ge,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1  
,d10,0\H,6,r11,2,a11,1,d11,0\H,7,r12,2,a12,1,d12,0\H,7,r13,2,a13,1,d13,0\H,7,r14,2,a14,  
1,d14,0\H,8,r15,2,a15,1,d15,0\H,8,r16,2,a16,1,d16,0\H,8,r17,2,a17,1,d17,0\r2=1.661358  
23\r3=1.21118342\r4=1.21139556\r5=1.21070704\r6=1.901097\r7=1.90099814\r8=1.90  
099107\r9=1.54748494\r10=1.53220434\r11=1.53720193\r12=1.54749145\r13=1.53251  
098\r14=1.53724621\r15=1.54765752\r16=1.53241957\r17=1.53726137\ a3=106.526932  
04\ a4=106.47354729\ a5=106.61709918\ a6=105.27772747\ a7=105.35589266\ a8=105.39  
81512\ a9=106.97975608\ a10=107.545671\ a11=106.20109743\ a12=106.89856324\ a13=1  
07.45393523\ a14=106.28305898\ a15=106.90167218\ a16=107.55619342\ a17=106.16359  
733\ d4=119.66545875\ d5=239.65375217\ d6=161.40369624\ d7=41.40067475\ d8=281.35  
720565\ d9=164.96571991\ d10=45.34301476\ d11=283.09896109\ d12=165.1194615\ d13  
=45.51093008\ d14=283.3382942\ d15=164.68703757\ d16=45.1498143\ d17=282.830299  
1\Version=EM64M-G09RevC.01\State=1-A\HF=-6291.0708929\RMSD=4.216e-  
09\RMSF=1.511e-  
04\Dipole=0.000002,0.0002421,1.5016369\Quadrupole=3.7902971,3.7956229,-  
7.58592,0.0009613,0.0090068,-0.0093021\PG=C01 [X(B1Ge3H12N1)]\@\n  
--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\B1Ge3H12N1\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
 geom=allcheck\title\0,1\B\N,1,1.661358228\H,1,1.2111834155,2,106.52693204\H,1,1.2113955611,2,106.47354729,3,119.66545875,0\H,1,1.2107070355,2,106.61709918,3,239.65375217,0\Ge,2,1.9010969954,1,105.27772747,3,161.40369624,0\Ge,2,1.9009981425,1,105.35589266,3,41.40067475,0\Ge,2,1.900991069,1,105.3981512,3,281.35720565,0\H,6,1.5474849351,2,106.97975608,1,164.96571991,0\H,6,1.5322043447,2,107.545671,1,45.34301476,0\H,6,1.5372019307,2,106.20109743,1,283.09896109,0\H,7,1.547491447,2,106.89856324,1,165.1194615,0\H,7,1.5325109827,2,107.45393523,1,45.51093008,0\H,7,1.5372462103,2,106.28305898,1,283.3382942,0\H,8,1.5476575211,2,106.90167218,1,164.68703757,0\H,8,1.5324195653,2,107.55619342,1,45.1498143,0\H,8,1.5372613671,2,106.16359733,1,282.8302991,0\Version=EM64M-G09RevC.01\State=1-A\HF=-6312.3713999\RMSD=5.353e-09\Dipole=0.000109,0.0004205,1.5703415\Quadrupole=3.8680862,3.8729812,-7.7410674,0.0018442,0.008896,-0.010793\PG=C01 [X(B1Ge3H12N1)]\@

HF=-6291.0708929

Sum of electronic and zero-point Energies= -6317.611845  
 Sum of electronic and thermal Energies= -6317.601334  
 Sum of electronic and thermal Enthalpies= -6317.600390  
 Sum of electronic and thermal Free Energies= -6317.648381  
 NImag=0

Ge3H9N1

-----  
 0,1  
 N  
 Ge,1,r2  
 Ge,1,r3,2,a3  
 Ge,1,r4,2,a4,3,d4,0  
 H,2,r5,1,a5,4,d5,0  
 H,2,r6,1,a6,4,d6,0  
 H,2,r7,1,a7,4,d7,0  
 H,3,r8,1,a8,2,d8,0  
 H,3,r9,1,a9,2,d9,0  
 H,3,r10,1,a10,2,d10,0  
 H,4,r11,1,a11,3,d11,0  
 H,4,r12,1,a12,3,d12,0  
 H,4,r13,1,a13,3,d13,0

r2=1.8466144  
 r3=1.84652173  
 r4=1.84642294  
 a3=119.8668485

a4=120.10046572  
d4=179.9695675  
r5=1.54563688  
r6=1.5459923  
r7=1.54559635  
a5=110.5812208  
a6=106.78129529  
a7=110.54642107  
d5=119.49234429  
d6=-0.21414381  
d7=240.07968849  
r8=1.54568323  
r9=1.54567312  
r10=1.54606695  
a8=110.61206714  
a9=110.62159205  
a10=106.73042931  
d8=240.14819363  
d9=119.56352716  
d10=-0.14573536  
r11=1.54556566  
r12=1.54605569  
r13=1.54561998  
a11=110.57073073  
a12=106.75582222  
a13=110.60084014  
d11=120.16239871  
d12=0.42728311  
d13=240.68528464

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\FOpt\RM062X\6-311++G(3df,2p)\Ge3H9N1\ROSMUSJ\17-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Ge,1,r2\Ge,1,r3,2,a3\Ge,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.8466144\r3=1.84652173\r4=1.84642294\a3=119.8668485\a4=120.10046572\d4=179.9695675\r5=1.54563688\r6=1.5459923\r7=1.54559635\a5=110.5812208\a6=106.78129529\a7=110.54642107\d5=119.49234429\d6=-0.21414381\d7=240.07968849\r8=1.54568323\r9=1.54567312\r10=1.54606695\a8=110.61206714\a9=110.62159205\a10=106.73042931\d8=240.14819363\d9=119.56352716\d10=-0.14573536\r11=1.54556566\r12=1.54605569\r13=1.54561998\a11=110.57073073\a12=106.75582222\a13=110.60084014\d11=120.16239871\d12=0.42728311\d13=240.68528464\Version=EM64M-G09RevC.01\State=1-A\HF=-6291.0780834\RMSD=5.106e-

09\RMSF=1.116e-04\Dipole=0.0001977,-0.000265,0.0002773\Quadrupole=0.4738051,-  
0.9565888,0.4827836,0.0032259,0.0034536,0.0017817\PG=C01 [X(Ge3H9N1)]\@  
--- NBO Single Point ---  
1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\Ge3H9N1\ROSMUSJ\18-Jun-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Ge,1,1.8466144007\Ge,1,1.8465217345,2,119.8668485\Ge,1  
,1.8464229426,2,120.10046572,3,179.9695675,0\H,2,1.5456368804,1,110.5812208,4,11  
9.49234429,0\H,2,1.5459923026,1,106.78129529,4,-  
0.21414381,0\H,2,1.5455963484,1,110.54642107,4,240.07968849,0\H,3,1.5456832345,1  
,110.61206714,2,240.14819363,0\H,3,1.5456731152,1,110.62159205,2,119.56352716,0\  
H,3,1.5460669522,1,106.73042931,2,-  
0.14573536,0\H,4,1.5455656563,1,110.57073073,3,120.16239871,0\H,4,1.5460556939,1  
,106.75582222,3,0.42728311,0\H,4,1.5456199833,1,110.60084014,3,240.68528464,0\|V  
ersion=EM64M-G09RevC.01\State=1-A\HF=-6285.9535765\RMSD=2.454e-  
09\Dipole=-0.000073,-0.0002627,-0.0000326\Quadrupole=0.3993037,-  
0.8072731,0.4079694,0.0029324,0.0042619,0.0014687\PG=C01 [X(Ge3H9N1)]\@

HF=-6291.0780834

Sum of electronic and zero-point Energies=	-6291.001484
Sum of electronic and thermal Energies=	-6290.992222
Sum of electronic and thermal Enthalpies=	-6290.991278
Sum of electronic and thermal Free Energies=	-6291.038886
NImag=0	

B1H6N1O1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
O,2,r6,1,a6,3,d6,0  
H,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0

r2=1.62427539  
r3=1.21041346  
r4=1.19983468  
r5=1.20000793  
r6=1.40332315  
r7=1.01833095  
r8=1.01825194

a3=101.23995432  
a4=105.4776888  
a5=105.43247159  
a6=112.65708268  
a7=108.45010755  
a8=108.6551664  
d4=118.82623222  
d5=241.34598169  
d6=179.79615229  
d7=59.14819199  
d8=300.55176056  
r9=0.964132  
a9=107.55892295  
d9=180.97826466

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1H6N1O1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\O,2,  
r6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\r2=1.62427539\r3  
=1.21041346\r4=1.19983468\r5=1.20000793\r6=1.40332315\r7=1.01833095\r8=1.01825  
194\ a3=101.23995432\ a4=105.4776888\ a5=105.43247159\ a6=112.65708268\ a7=108.45  
010755\ a8=108.6551664\ d4=118.82623222\ d5=241.34598169\ d6=179.79615229\ d7=59.  
14819199\ d8=300.55176056\ r9=0.964132\ a9=107.55892295\ d9=180.97826466\ Version  
=EM64M-G09RevC.01\State=1-A\HF=-131.706228\RMSD=2.144e-09\RMSF=9.958e-  
05\Dipole=0.5169043,0.0089667,2.3320149\Quadrupole=-  
0.6102647,0.2376506,0.3726142,-0.0136243,1.2830521,0.0366363\PG=C01  
[X(B1H6N1O1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1H6N1O1\ROSMUSJ\14-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6242753945\H,1,1.210413464,2,101.23995432\H,1,1.1  
998346802,2,105.4776888,3,118.82623222,0\H,1,1.2000079301,2,105.43247159,3,241.3  
4598169,0\O,2,1.40332315,1,112.65708268,3,179.79615229,0\H,2,1.0183309501,1,108.  
45010755,3,59.14819199,0\H,2,1.018251939,1,108.6551664,3,300.55176056,0\H,6,0.96  
41319981,2,107.55892295,1,180.97826466,0\Version=EM64M-G09RevC.01\State=1-  
A\HF=-157.4805317\RMSD=8.664e-  
09\Dipole=0.5360356,0.0090179,2.4387473\Quadrupole=-  
0.6676734,0.3541938,0.3134796,-0.0143526,1.4154515,0.0368678\PG=C01  
[X(B1H6N1O1)]\@

HF=-131.706228

Sum of electronic and zero-point Energies= -158.276811  
Sum of electronic and thermal Energies= -158.272251

Sum of electronic and thermal Enthalpies= -158.271307  
Sum of electronic and thermal Free Energies= -158.302429  
NImag=0

H3N1O1

-----  
0,1  
N  
O,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0

r2=1.42017183  
r3=1.0154182  
r4=1.01539047  
r5=0.95868095  
a3=104.68557609  
a4=104.66693519  
a5=103.47281683  
d4=111.41687874  
d5=235.70451328

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1O1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\O,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\r2=1.42017183  
\r3=1.0154182\r4=1.01539047\r5=0.95868095\a3=104.68557609\a4=104.66693519\a5=  
103.47281683\d4=111.41687874\d5=235.70451328\Version=EM64M-  
G09RevC.01\State=1-A\HF=-131.712902\RMSD=2.597e-09\RMSF=2.762e-  
05\Dipole=0.0177511,-0.0259343,-0.2218144\Quadrupole=0.2474612,0.3405543,-  
0.5880154,-0.1179826,-1.6067999,2.355716\PG=C01 [X(H3N1O1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\H3N1O1\ROSMUSJ\14-Jun-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\O,1,1.4201718338\H,1,1.0154181984,2,104.68557609\H,1,1  
.0153904738,2,104.66693519,3,111.41687874,0\H,2,0.9586809457,1,103.47281683,4,23  
5.70451328,0\Version=EM64M-G09RevC.01\State=1-A\HF=-  
131.053276\RMSD=5.451e-09\Dipole=0.0167843,-0.0245104,-  
0.2566194\Quadrupole=0.2868839,0.3853489,-0.6722328,-0.1248498,-  
1.6324423,2.3933056\PG=C01 [X(H3N1O1)]\@

HF=-131.712902

Sum of electronic and zero-point Energies= -131.671805

Sum of electronic and thermal Energies= -131.668647  
Sum of electronic and thermal Enthalpies= -131.667703  
Sum of electronic and thermal Free Energies= -131.694209  
NImag=0

B1H6N1O2

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
O,2,r6,1,a6,3,d6,0  
O,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,7,r10,2,a10,1,d10,0

r2=1.62982276  
r3=1.20179499  
r4=1.20254077  
r5=1.19679243  
r6=1.38717358  
r7=1.38761791  
r8=1.02179289  
a3=102.46287122  
a4=102.23635735  
a5=104.81450684  
a6=110.88467  
a7=110.77601566  
a8=107.82855031  
d4=118.11507839  
d5=238.9230429  
d6=182.02020187  
d7=58.93508216  
d8=300.59802259  
r9=0.96604099  
r10=0.96620489  
a9=108.1235514  
a10=107.94550019  
d9=166.63947397  
d10=185.30098385

--- Geometry Optimization ---



```

1\1\GINC-MH325M15MH\FOpt\RM062X\6-
311++G(3df,2p)\B1H6N1O2\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p)
opt=(z-matrix,noeigen) optcyc=100 freq
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\O,2,
r6,1,a6,3,d6,0\O,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,7,r10,2,a10,1,d1
0,0\r2=1.62982276\r3=1.20179499\r4=1.20254077\r5=1.19679243\r6=1.38717358\r7=1
.38761791\r8=1.02179289\a3=102.46287122\a4=102.23635735\a5=104.81450684\a6=1
10.88467\a7=110.77601566\a8=107.82855031\d4=118.11507839\d5=238.9230429\d6=1
82.02020187\d7=58.93508216\d8=300.59802259\r9=0.96604099\r10=0.96620489\a9=1
08.1235514\a10=107.94550019\d9=166.63947397\d10=185.30098385\Version=EM64
M-G09RevC.01\State=1-A\HF=-206.8827497\RMSD=8.894e-09\RMSF=1.573e-
04\Dipole=0.2704681,-0.5490601,2.6749942\Quadrupole=-1.197551,-
0.3108364,1.5083875,-0.4842916,0.5849451,-1.2685284\PG=C01 [X(B1H6N1O2)]\@
--- NBO Single Point ---
1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1H6N1O2\ROSMUSJ\18-Jun-
2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\title\0,1\B\N,1,1.6298227639\H,1,1.2017949879,2,102.46287122\H,1,1.
2025407734,2,102.23635735,3,118.11507839,0\H,1,1.1967924307,2,104.81450684,3,23
8.9230429,0\O,2,1.3871735833,1,110.88467,3,182.02020187,0\O,2,1.3876179084,1,110.
77601566,3,58.93508216,0\H,2,1.0217928859,1,107.82855031,3,300.59802259,0\H,6,0.
9660409931,2,108.1235514,1,166.63947397,0\H,7,0.9662048885,2,107.94550019,1,185.
30098385,0\Version=EM64M-G09RevC.01\State=1-A\HF=-
232.3139405\RMSD=7.282e-09\Dipole=0.2901607,-0.5827771,2.8064205\Quadrupole=-
1.2568297,-0.2354934,1.4923231,-0.5974708,0.6380642,-1.3575666\PG=C01
[X(B1H6N1O2)]\@

```

HF=-206.8827497

```

Sum of electronic and zero-point Energies=      -233.443547
Sum of electronic and thermal Energies=         -233.438001
Sum of electronic and thermal Enthalpies=       -233.437057
Sum of electronic and thermal Free Energies=    -233.471244
NImag=0

```

H3N1O2

```

-----
0,1
N
O,1,r2
O,1,r3,2,a3
H,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,3,r6,1,a6,2,d6,0

```

r2=1.40304765

r3=1.40256956  
r4=1.01568869  
r5=0.96014904  
r6=0.96020328  
a3=107.59982941  
a4=101.91278789  
a5=104.24794641  
a6=104.2594595  
d4=106.63433908  
d5=214.38719025  
d6=252.56534258

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1O2\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\O,1,r2\O,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\|r2=1.40304765|r3=1.40256956|r4=1.01568869|r5=0.96014904|r6=0.96020328|a3=107.59982941|a4=101.91278789|a5=104.24794641|a6=104.2594595|d4=106.63433908|d5=214.38719025|d6=252.56534258\|Version=EM64M-G09RevC.01\State=1-A\HF=-206.8949635\RMSD=4.320e-09\RMSF=1.335e-04\Dipole=-0.2674,0.5935155,-0.1946935\Quadrupole=-1.3039686,2.0074426,-0.703474,1.4603806,-0.9696154,1.0721465\PG=C01 [X(H3N1O2)]\|@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\H3N1O2\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\O,1,1.4030476489\O,1,1.4025695638,2,107.59982941\H,1,1.0156886861,2,101.91278789,3,106.63433908,0\H,2,0.9601490387,1,104.24794641,4,214.38719025,0\H,3,0.9602032803,1,104.2594595,2,252.56534258,0\|Version=EM64M-G09RevC.01\State=1-A\HF=-205.8998851\RMSD=2.576e-09\Dipole=-0.3050822,0.6173939,-0.2221647\Quadrupole=-1.3260868,2.1079204,-0.7818336,1.4927494,-0.8816197,1.0958784\PG=C01 [X(H3N1O2)]\|@

HF=-206.8949635

Sum of electronic and zero-point Energies=	-206.849019
Sum of electronic and thermal Energies=	-206.845226
Sum of electronic and thermal Enthalpies=	-206.844282
Sum of electronic and thermal Free Energies=	-206.873843

NImag=0

B1H6N1O3

-----  
0,1  
B  
N,1,r2

H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
O,2,r6,1,a6,3,d6,0  
O,2,r7,1,a7,3,d7,0  
O,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,7,r10,2,a10,1,d10,0  
H,8,r11,2,a11,1,d11,0

r2=1.63714548  
r3=1.19293406  
r4=1.2030862  
r5=1.20660952  
r6=1.38994825  
r7=1.37935219  
r8=1.36774932  
a3=105.1199273  
a4=103.28743096  
a5=101.01995474  
a6=111.80202629  
a7=112.90387038  
a8=111.90349889  
d4=121.56362085  
d5=239.66936045  
d6=188.29368684  
d7=69.60235892  
d8=309.53222393  
r9=0.96892398  
r10=0.96858085  
r11=0.96987536  
a9=103.04793819  
a10=103.47105551  
a11=105.14264142  
d9=383.1588167  
d10=382.31626819  
d11=182.84121326

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\B1H6N1O3\ROSMUS\30-Jan-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100 freq counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\O,2,r6,1,a6,3,d6,0\O,2,r7,1,a7,3,d7,0\O,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,7,r10,2,a10,1,d10,0\H,8,r11,2,a11,1,d11,0\r2=1.63714548\r3=1.19293406\r4=1.2030862\r5=1.20660952\r6=1.38994825\r7=1.37935219\r8=1.36774932\a3=105.1199273\a4=103.28743096\a5=101.01995474\a6=111.80202629\a7=112.90387038\a8=111.90349889\d4=121.56362085

\d5=239.66936045\d6=188.29368684\d7=69.60235892\d8=309.53222393\r9=0.9689239  
8\r10=0.96858085\r11=0.96987536\a9=103.04793819\a10=103.47105551\a11=105.1426  
4142\d9=383.1588167\d10=382.31626819\d11=182.84121326\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-282.082838\RMSD=5.282e-09\RMSF=9.563e-  
05\Dipole=-0.3606136,0.1169123,0.8915048\Quadrupole=0.1999963,1.8471614,-  
2.0471577,1.44606,1.9013835,-2.157272\PG=C01 [X(B1H6N1O3)]\@\n  
--- NBO Single Point ---

HF=-307.1805668

Sum of electronic and zero-point Energies=	-307.092149
Sum of electronic and thermal Energies=	-307.086913
Sum of electronic and thermal Enthalpies=	-307.085969
Sum of electronic and thermal Free Energies=	-307.120036
NImag=0	

H3N1O3

-----  
0,1  
N  
O,1,r2  
O,1,r3,2,a3  
O,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0  
H,4,r7,1,a7,3,d7,0

r2=1.39272034  
r3=1.39265344  
r4=1.39257889  
r5=0.96226743  
r6=0.96231784  
r7=0.96249095  
a3=103.65904918  
a4=103.67030219  
a5=103.5224543  
a6=103.53619422  
a7=103.53106421  
d4=108.01273066  
d5=206.08017922  
d6=205.43821199  
d7=205.94728584

--- Geometry Optimization ---

```

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1O3\ROSMUSJ\15-
Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\N\O,1,r2\O,1,r3,2,a3\O,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6
,0\H,4,r7,1,a7,3,d7,0\r2=1.39272034\r3=1.39265344\r4=1.39257889\r5=0.96226743\r6=
0.96231784\r7=0.96249095\a3=103.65904918\a4=103.67030219\a5=103.5224543\a6=1
03.53619422\a7=103.53106421\d4=108.01273066\d5=206.08017922\d6=205.43821199\
d7=205.94728584\Version=EM64M-G09RevC.01\State=1-A\HF=-
282.0794705\RMSD=2.175e-09\RMSF=8.902e-05\Dipole=-0.6498316,0.8869217,-
0.511352\Quadrupole=0.1640488,-0.7108367,0.5467879,1.2992655,-
0.7615303,1.0480439\PG=C01 [X(H3N1O3)]\@
--- NBO Single Point ---
1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\H3N1O3\ROSMUSJ\18-Jun-2012\0\#p
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\title\0,1\N\O,1,1.3927204919\O,1,1.3926534804,2,103.65909354\O,1,1
.3925787978,2,103.67028112,3,108.01268444,0\H,2,0.9622674271,1,103.52246625,4,20
6.08035498,0\H,3,0.9623177388,1,103.53619662,2,205.43847025,0\H,4,0.962491042,1,
103.53106948,3,205.94725666,0\Version=EM64M-G09RevC.01\State=1-A\HF=-
280.7485633\RMSD=3.271e-09\Dipole=-0.6910113,0.9435317,-
0.5437855\Quadrupole=0.157319,-0.6803359,0.5230169,1.2412136,-
0.7285759,1.0023525\PG=C01 [X(H3N1O3)]\@

```

HF=-282.0794705

```

Sum of electronic and zero-point Energies=      -282.030759
Sum of electronic and thermal Energies=         -282.025777
Sum of electronic and thermal Enthalpies=       -282.024833
Sum of electronic and thermal Free Energies=     -282.057822
NImag=0

```

B1H6N1Se1

```

-----
0,1
B
N,1,r2
H,1,r3,2,a3
H,1,r4,2,a4,3,d4,0
H,1,r5,2,a5,3,d5,0
Se,2,r6,1,a6,3,d6,0
H,2,r7,1,a7,3,d7,0
H,2,r8,1,a8,3,d8,0
H,6,r9,2,a9,1,d9,0

```

```

r2=1.64906938
r3=1.2048368
r4=1.20386873

```

r5=1.20398927  
r6=1.8875004  
r7=1.01521945  
r8=1.01502585  
a3=103.94825563  
a4=104.89675702  
a5=104.88912857  
a6=110.51041829  
a7=108.99986982  
a8=108.96441263  
d4=120.16093022  
d5=240.28827028  
d6=178.84485402  
d7=58.16529545  
d8=299.52787344  
r9=1.47229459  
a9=95.43340523  
d9=179.26532385

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1H6N1Se1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Se,2,  
r6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\r2=1.64906938\r3  
=1.2048368\r4=1.20386873\r5=1.20398927\r6=1.8875004\r7=1.01521945\r8=1.0150258  
5\a3=103.94825563\a4=104.89675702\a5=104.88912857\a6=110.51041829\a7=108.999  
86982\a8=108.96441263\d4=120.16093022\d5=240.28827028\d6=178.84485402\d7=58.  
16529545\d8=299.52787344\r9=1.47229459\a9=95.43340523\d9=179.26532385\Version  
=EM64M-G09RevC.01\State=1-A\HF=-2458.0825554\RMSD=3.772e-  
09\RMSF=2.320e-04\Dipole=0.117648,-  
0.0059147,2.0427731\Quadrupole=3.0041925,0.4928397,-3.4970322,-  
0.0549795,3.8443496,-0.1118354\PG=C01 [X(B1H6N1Se1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1H6N1Se1\ROSMUSJ\14-Jun-  
2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6490693817\H,1,1.2048368008,2,103.94825563\H,1,1.  
2038687323,2,104.89675702,3,120.16093022,0\H,1,1.203989271,2,104.88912857,3,240.  
28827028,0\Se,2,1.8875004017,1,110.51041829,3,178.84485402,0\H,2,1.0152194503,1,  
108.99986982,3,58.16529545,0\H,2,1.0150258494,1,108.96441263,3,299.52787344,0\H,  
6,1.472294585,2,95.43340523,1,179.26532385,0\Version=EM64M-  
G09RevC.01\State=1-A\HF=-2482.5189938\RMSD=3.064e-09\Dipole=0.1222861,-  
0.0068072,2.1322037\Quadrupole=3.0101205,0.6218709,-3.6319914,-  
0.0537161,4.0616351,-0.1142412\PG=C01 [X(B1H6N1Se1)]\@

HF=-2458.0825554

Sum of electronic and zero-point Energies= -2484.655553  
 Sum of electronic and thermal Energies= -2484.650403  
 Sum of electronic and thermal Enthalpies= -2484.649459  
 Sum of electronic and thermal Free Energies= -2484.683971  
 NImag=0

H3N1Se1

-----  
 0,1  
 N  
 Se,1,r2  
 H,1,r3,2,a3  
 H,1,r4,2,a4,3,d4,0  
 H,2,r5,1,a5,4,d5,0

r2=1.85574312  
 r3=1.01117323  
 r4=1.01117423  
 r5=1.46906628  
 a3=109.39307571  
 a4=109.39320483  
 a5=95.18164948  
 d4=119.1446478  
 d5=239.60818327

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1Se1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
 freq\title\0,1\N\Se,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\r2=1.8557431  
 2\r3=1.01117323\r4=1.01117423\r5=1.46906628\a3=109.39307571\a4=109.39320483\a  
 5=95.18164948\d4=119.1446478\d5=239.60818327\Version=EM64M-  
 G09RevC.01\State=1-A\HF=-2458.0838813\RMSD=3.438e-09\RMSF=3.555e-  
 05\Dipole=0.140723,-0.2398363,-0.2551674\Quadrupole=-0.6049861,-  
 0.0610509,0.666037,-0.4914633,-1.3891017,2.3645223\PG=C01 [X(H3N1Se1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\H3N1Se1\ROSMUSJ\14-Jun-2012\0\#p  
 hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
 geom=allcheck\title\0,1\N\Se,1,1.8557431234\H,1,1.0111732282,2,109.39307571\H,1,  
 1.0111742333,2,109.39320483,3,119.1446478,0\H,2,1.4690662804,1,95.18164948,4,239  
 .60818327,0\Version=EM64M-G09RevC.01\State=1-A\HF=-  
 2456.0921547\RMSD=9.572e-09\Dipole=0.1446556,-0.2465709,-  
 0.2623594\Quadrupole=-0.5992941,-0.0081376,0.6074317,-0.5338695,-  
 1.4402093,2.4514342\PG=C01 [X(H3N1Se1)]\@

HF=-2458.0838813

Sum of electronic and zero-point Energies= -2458.049573  
Sum of electronic and thermal Energies= -2458.046126  
Sum of electronic and thermal Enthalpies= -2458.045182  
Sum of electronic and thermal Free Energies= -2458.074701  
NImag=0

B1H6N1Se2

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Se,2,r6,1,a6,3,d6,0  
Se,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,7,r10,2,a10,1,d10,0

r2=1.66286579  
r3=1.20363517  
r4=1.20365307  
r5=1.2029118  
r6=1.88930151  
r7=1.88955888  
r8=1.01548967  
a3=104.0610326  
a4=104.09708273  
a5=104.53576123  
a6=107.6645979  
a7=107.46893972  
a8=106.93896212  
d4=119.70596777  
d5=239.83231739  
d6=185.21596456  
d7=57.58691503  
d8=301.46863338  
r9=1.47343224  
r10=1.47331396  
a9=94.97070264  
a10=95.01763466  
d9=183.26046317



d10=177.1586216

--- Geometry Optimization ---

```
1\1\GINC-MH325M15MH\FOpt\RM062X\6-
311++G(3df,2p)\B1H6N1Se2\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p)
opt=(z-matrix,noeigen) optcyc=100 freq
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Se,2,
r6,1,a6,3,d6,0\Se,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,7,r10,2,a10,1,d
10,0\r2=1.66286579\r3=1.20363517\r4=1.20365307\r5=1.2029118\r6=1.88930151\r7=1
.88955888\r8=1.01548967\a3=104.0610326\a4=104.09708273\a5=104.53576123\a6=10
7.6645979\a7=107.46893972\a8=106.93896212\d4=119.70596777\d5=239.83231739\d6
=185.21596456\d7=57.58691503\d8=301.46863338\r9=1.47343224\r10=1.47331396\a9
=94.97070264\a10=95.01763466\d9=183.26046317\d10=177.1586216\Version=EM64
M-G09RevC.01\State=1-A\HF=-4859.6171576\RMSD=7.946e-09\RMSF=7.667e-
05\Dipole=0.0153607,-0.021542,2.024434\Quadrupole=1.9029956,0.7771812,-
2.6801768,1.1003315,0.7888615,-1.2835016\PG=C01 [X(B1H6N1Se2)]\@
```

--- NBO Single Point ---

```
1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1H6N1Se2\ROSMUSJ\18-Jun-
2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\title\0,1\B\N,1,1.6628657928\H,1,1.2036351748,2,104.0610326\H,1,1.2
03653072,2,104.09708273,3,119.70596777,0\H,1,1.2029117951,2,104.53576123,3,239.8
3231739,0\Se,2,1.8893015074,1,107.6645979,3,185.21596456,0\Se,2,1.8895588797,1,1
07.46893972,3,57.58691503,0\H,2,1.0154896672,1,106.93896212,3,301.46863338,0\H,6
,1.4734322419,2,94.97070264,1,183.26046317,0\H,7,1.4733139569,2,95.01763466,1,17
7.1586216,0\Version=EM64M-G09RevC.01\State=1-A\HF=-
4882.3774845\RMSD=4.494e-09\Dipole=0.019885,-
0.028659,2.1314467\Quadrupole=1.8957694,0.8747529,-2.7705223,0.996735,0.858037,-
1.3957816\PG=C01 [X(B1H6N1Se2)]\@
```

HF=-4859.6171576

Sum of electronic and zero-point Energies=	-4886.187988
Sum of electronic and thermal Energies=	-4886.181607
Sum of electronic and thermal Enthalpies=	-4886.180662
Sum of electronic and thermal Free Energies=	-4886.219793
NImag=0	

H3N1Se2

-----  
0,1  
N  
Se,1,r2  
Se,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0

H,3,r6,1,a6,2,d6,0

r2=1.84592546  
r3=1.84594325  
r4=1.00879659  
r5=1.47141754  
r6=1.47141869  
a3=120.66809104  
a4=111.0932537  
a5=95.34705595  
a6=95.34715183  
d4=132.61995061  
d5=244.24627018  
d6=248.36751306

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1Se2\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Se,1,r2\Se,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\r2=1.84592546\r3=1.84594325\r4=1.00879659\r5=1.47141754\r6=1.47141869\a3=120.66809104\a4=111.0932537\a5=95.34705595\a6=95.34715183\d4=132.61995061\d5=244.24627018\d6=248.36751306\Version=EM64M-G09RevC.01\State=1-A\HF=-4859.6173158\RMSD=3.768e-09\RMSF=9.222e-05\Dipole=-0.2228083,0.0970864,-0.1269219\Quadrupole=-1.0491383,1.1776502,-0.1285119,0.2525111,-0.7758702,0.1437757\PG=C01 [X(H3N1Se2)]\@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\H3N1Se2\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Se,1,1.8459254629\Se,1,1.8459432504,2,120.66809104\H,1,1.008796592,2,111.0932537,3,132.61995061,0\H,2,1.4714175446,1,95.34705595,4,244.24627018,0\H,3,1.4714186909,1,95.34715183,2,248.36751306,0\Version=EM64M-G09RevC.01\State=1-A\HF=-4855.9584221\RMSD=3.378e-09\Dipole=-0.2364156,0.1096945,-0.1346814\Quadrupole=-1.0875892,1.2866871,-0.1990979,0.2741306,-0.7487456,0.1560958\PG=C01 [X(H3N1Se2)]\@

HF=-4859.6173158

Sum of electronic and zero-point Energies= -4859.584730  
Sum of electronic and thermal Energies= -4859.579952  
Sum of electronic and thermal Enthalpies= -4859.579008  
Sum of electronic and thermal Free Energies= -4859.614352  
NImag=0

B1H6N1Se3

-----

0,1  
B  
N,1,rN  
H,1,rB,2,aB  
H,1,rB,2,aB,3,120.,0  
H,1,rB,2,aB,3,-120.,0  
Se,2,rS,1,aS,3,180.,0  
Se,2,rS,1,aS,3,60.,0  
Se,2,rS,1,aS,3,-60.,0  
H,6,rH,2,aH,1,180.,0  
H,7,rH,2,aH,1,180.,0  
H,8,rH,2,aH,1,180.,0

rN=1.68794154  
rB=1.20247079  
rS=1.90380035  
aB=103.94200791  
aS=104.37383001  
rH=1.4741762  
aH=94.34594556

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\B1H6N1Se3\ROSMUSJ\15-Jun-2012\1\#\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,rN\H,1,rB,2,aB\H,1,rB,2,aB,3,120.,0\H,1,rB,2,aB,3,-120.,0\Se,2,rS,1,aS,3,180.,0\Se,2,rS,1,aS,3,60.,0\Se,2,rS,1,aS,3,-60.,0\H,6,rH,2,aH,1,180.,0\H,7,rH,2,aH,1,180.,0\H,8,rH,2,aH,1,180.,0\rN=1.68794154\rB=1.20247079\rS=1.90380035\aB=103.94200791\aS=104.37383001\rH=1.4741762\aH=94.34594556\Version=EM64M-G09RevC.01\State=1-A1\HF=-7261.1483627\RMSD=7.957e-09\RMSF=7.108e-06\Dipole=0.,0.,2.0113387\Quadrupole=0.7984191,0.7984191,-1.5968382,0.,0.,0.\PG=C03V [C3(N1B1),3SGV(H2Se1)]\@\

--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\B1H6N1Se3\ROSMUSJ\18-Jun-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6879417369\H,1,1.2024707768,2,103.94200665\H,1,1.2024707768,2,103.94200665,3,120.,0\H,1,1.2024707768,2,103.94200665,3,-120.,0\Se,2,1.9038003149,1,104.37382372,3,180.,0\Se,2,1.9038003149,1,104.37382372,3,60.,0\Se,2,1.9038003149,1,104.37382372,3,-60.,0\H,6,1.4741762136,2,94.34594743,1,180.,0\H,7,1.4741762136,2,94.34594743,1,180.,0\H,8,1.4741762136,2,94.34594743,1,180.,0\Version=EM64M-G09RevC.01\State=1-A1\HF=-7282.2292633\RMSD=3.389e-09\Dipole=0.,0.,2.1227484\Quadrupole=0.7994801,0.7994801,-1.5989603,0.,0.,0.\PG=C03V [C3(N1B1),3SGV(H2Se1)]\@\

HF=-7261.1483627

Sum of electronic and zero-point Energies= -7287.719194  
Sum of electronic and thermal Energies= -7287.710623  
Sum of electronic and thermal Enthalpies= -7287.709679  
Sum of electronic and thermal Free Energies= -7287.753402  
NImag=0

H3N1Se3

-----  
0,1  
N  
X,1,1.  
Se,1,rS,2,aS  
Se,1,rS,2,aS,3,dS,0  
Se,1,rS,2,aS,3,-dS,0  
H,3,rH,1,aH,2,dH,0  
H,4,rH,1,aH,2,dH,0  
H,5,rH,1,aH,2,dH,0

rS=1.8524008  
rH=1.47803171  
aS=98.624039  
aH=97.14220715  
dS=120.  
dH=180.

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1Se3\ROSMUSJ\15-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\X,1,1.\Se,1,rS,2,aS\Se,1,rS,2,aS,3,dS,0\Se,1,rS,2,aS,3,-  
dS,0\H,3,rH,1,aH,2,dH,0\H,4,rH,1,aH,2,dH,0\H,5,rH,1,aH,2,dH,0\rS=1.8524008\rH=1.4  
7803171\aS=98.624039\aH=97.14220715\dS=120.\dH=180.\Version=EM64M-  
G09RevC.01\State=1-A1\HF=-7261.1519545\RMSD=7.257e-09\RMSF=3.660e-  
05\Dipole=0.,0.,-0.681799\Quadrupole=-1.2384551,-  
1.2384551,2.4769102,0.,0.,0.\PG=C03V [C3(N1),3SGV(H1Se1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\H3N1Se3\ROSMUSJ\18-Jun-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\X,1,1.\Se,1,1.8524007976,2,98.62403914\Se,1,1.852400797  
6,2,98.62403914,3,120.,0\Se,1,1.8524007976,2,98.62403914,3,-  
120.,0\H,3,1.478031713,1,97.14220728,2,180.,0\H,4,1.478031713,1,97.14220728,2,180.,  
0\H,5,1.478031713,1,97.14220728,2,180.,0\Version=EM64M-G09RevC.01\State=1-  
A1\HF=-7255.8230303\RMSD=9.626e-09\Dipole=0.,0.,-0.7400893\Quadrupole=-  
1.4013811,-1.4013811,2.8027622,0.,0.,0.\PG=C03V [C3(N1),3SGV(H1Se1)]\@

HF=-7261.1519545

Sum of electronic and zero-point Energies= -7261.122522  
Sum of electronic and thermal Energies= -7261.115566  
Sum of electronic and thermal Enthalpies= -7261.114622  
Sum of electronic and thermal Free Energies= -7261.155372  
NImag=0

B1H8N1Si1

-----

0,1

B

N,1,r2

H,1,r3,2,a3

H,1,r4,2,a4,3,d4,0

H,1,r5,2,a5,3,d5,0

Si,2,r6,1,a6,3,d6,0

H,2,r7,1,a7,3,d7,0

H,2,r8,1,a8,3,d8,0

H,6,r9,2,a9,1,d9,0

H,6,r10,2,a10,1,d10,0

H,6,r11,2,a11,1,d11,0

r2=1.66524679

r3=1.20209728

r4=1.20398462

r5=1.20994652

r6=1.79281933

r7=1.01638544

r8=1.01564299

r9=1.47700106

r10=1.4645397

r11=1.46686301

a3=106.45215675

a4=104.72380765

a5=104.4632782

a6=107.63262354

a7=108.40322588

a8=108.75665672

a9=108.30223281

a10=107.61206215

a11=106.23214253

d4=121.38140758

d5=239.86511023

d6=162.43861378  
d7=41.57287944  
d8=286.1559521  
d9=166.381115  
d10=46.68418286  
d11=284.7247745

--- Geometry Optimization ---

```
1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\B1H8N1Si1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p)
opt=(calcfc,z-matrix,noeigen) optcyc=100 freq
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Si,2,
r6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d1
0,0\H,6,r11,2,a11,1,d11,0\r2=1.66524679\r3=1.20209728\r4=1.20398462\r5=1.2099465
2\r6=1.79281933\r7=1.01638544\r8=1.01564299\r9=1.47700106\r10=1.4645397\r11=1.
46686301\a3=106.45215675\a4=104.72380765\a5=104.4632782\a6=107.63262354\a7=1
08.40322588\a8=108.75665672\a9=108.30223281\a10=107.61206215\a11=106.2321425
3\d4=121.38140758\d5=239.86511023\d6=162.43861378\d7=41.57287944\d8=286.1559
521\d9=166.381115\d10=46.68418286\d11=284.7247745\Version=EM64M-
G09RevC.01\State=1-A\HF=-347.2430463\RMSD=2.055e-09\RMSF=2.725e-
05\Dipole=-0.078248,0.0324339,1.8195544\Quadrupole=2.31501,1.7006013,-
4.0156112,-0.2231116,3.1482927,-0.9306044\PG=C01 [X(B1H8N1Si1)]\@
```

--- NBO Single Point ---

```
1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1H8N1Si1\ROSMUSJ\14-Jun-
2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read
geom=allcheck\title\0,1\B\N,1,1.6652467938\H,1,1.2020972789,2,106.45215675\H,1,1.
2039846228,2,104.72380765,3,121.38140758,0\H,1,1.2099465229,2,104.4632782,3,239.
86511023,0\Si,2,1.7928193272,1,107.63262354,3,162.43861378,0\H,2,1.0163854394,1,
108.40322588,3,41.57287944,0\H,2,1.0156429924,1,108.75665672,3,286.1559521,0\H,6
,1.4770010635,2,108.30223281,1,166.381115,0\H,6,1.4645397022,2,107.61206215,1,46.
68418286,0\H,6,1.4668630146,2,106.23214253,1,284.7247745,0\Version=EM64M-
G09RevC.01\State=1-A\HF=-372.7846892\RMSD=9.517e-09\Dipole=-
0.0626797,0.0249252,1.8770025\Quadrupole=2.3764816,1.775197,-4.1516785,-
0.225714,3.3050008,-0.9783307\PG=C01 [X(B1H8N1Si1)]\@
```

HF=-347.2430463

Sum of electronic and zero-point Energies=	-373.801099
Sum of electronic and thermal Energies=	-373.795497
Sum of electronic and thermal Enthalpies=	-373.794553
Sum of electronic and thermal Free Energies=	-373.828738
NImag=0	

H5N1Si1

-----

0,1  
N  
Si,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.71981477  
r3=1.00769422  
r4=1.00767766  
a3=120.35770034  
a4=120.13252316  
d4=144.13539606  
r5=1.48280262  
r6=1.47568219  
r7=1.47572915  
a5=115.35968054  
a6=107.72589283  
a7=108.0266323  
d5=73.84500433  
d6=-46.38260215  
d7=194.07839365

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\H5N1Si1\ROSMUSJ\14-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Si,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.71981477\r3=1.00769422\r4=1.00767766\ a3=120.35770034  
\a4=120.13252316\d4=144.13539606\r5=1.48280262\r6=1.47568219\r7=1.47572915\ a5  
=115.35968054\ a6=107.72589283\ a7=108.0266323\d5=73.84500433\d6=-  
46.38260215\d7=194.07839365\Version=EM64M-G09RevC.01\State=1-A\HF=-  
347.2470696\RMSD=9.425e-09\RMSF=3.004e-05\Dipole=0.0863029,-0.2662199,-  
0.3696006\Quadrupole=0.5580104,-1.4472234,0.889213,0.7275637,-  
0.4393357,1.3036003\PG=C01 [X(H5N1Si1)]\@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\H5N1Si1\ROSMUSJ\14-Jun-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\Si,1,1.7198147689\H,1,1.0076942205,2,120.35770034\H,1,1  
.0076776641,2,120.13252316,3,144.13539606,0\H,2,1.482802624,1,115.35968054,4,73.  
84500433,0\H,2,1.4756821937,1,107.72589283,4,-  
46.38260215,0\H,2,1.4757291482,1,108.0266323,4,194.07839365,0\Version=EM64M-  
G09RevC.01\State=1-A\HF=-346.359791\RMSD=2.651e-09\Dipole=0.0922606,-  
0.2841081,-0.3913195\Quadrupole=0.5342919,-1.4063382,0.8720463,0.704203,-  
0.4498358,1.3349658\PG=C01 [X(H5N1Si1)]\@

HF=-347.2470696

Sum of electronic and zero-point Energies= -347.196506  
Sum of electronic and thermal Energies= -347.192226  
Sum of electronic and thermal Enthalpies= -347.191282  
Sum of electronic and thermal Free Energies= -347.221326  
NImag=0

B1H10N1Si2

-----

0,1

B

N,1,r2

H,1,r3,2,a3

H,1,r4,2,a4,3,d4,0

H,1,r5,2,a5,3,d5,0

Si,2,r6,1,a6,3,d6,0

Si,2,r7,1,a7,3,d7,0

H,2,r8,1,a8,3,d8,0

H,6,r9,2,a9,1,d9,0

H,6,r10,2,a10,1,d10,0

H,6,r11,2,a11,1,d11,0

H,7,r12,2,a12,1,d12,0

H,7,r13,2,a13,1,d13,0

H,7,r14,2,a14,1,d14,0

r2=1.68089367

r3=1.20754403

r4=1.20152276

r5=1.20914166

r6=1.78601567

r7=1.78817402

r8=1.01777503

r9=1.47759452

r10=1.46637377

r11=1.4699688

r12=1.47946367

r13=1.46600408

r14=1.46767376

a3=106.04157348

a4=105.95381777

a5=104.24495926

a6=105.74623825

a7=105.42640149



a8=107.30651279  
a9=107.97297887  
a10=109.14774163  
a11=105.8524078  
a12=107.89916974  
a13=107.36840081  
a14=107.66869623  
d4=121.32457802  
d5=241.18987833  
d6=158.03994471  
d7=33.18444321  
d8=276.44982607  
d9=164.31501477  
d10=44.1044687  
d11=281.99899809  
d12=166.53194298  
d13=47.87987524  
d14=285.24437791

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1H10N1Si2\ROSMUSJ\16-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Si,2,  
r6,1,a6,3,d6,0\Si,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d  
0,0\H,6,r11,2,a11,1,d11,0\H,7,r12,2,a12,1,d12,0\H,7,r13,2,a13,1,d13,0\H,7,r14,2,a14,1,d  
14,0\r2=1.68089367\r3=1.20754403\r4=1.20152276\r5=1.20914166\r6=1.78601567\r7=  
1.78817402\r8=1.01777503\r9=1.47759452\r10=1.46637377\r11=1.4699688\r12=1.4794  
6367\r13=1.46600408\r14=1.46767376\A3=106.04157348\A4=105.95381777\A5=104.244  
95926\A6=105.74623825\A7=105.42640149\A8=107.30651279\A9=107.97297887\A10=10  
9.14774163\A11=105.8524078\A12=107.89916974\A13=107.36840081\A14=107.6686962  
3\d4=121.32457802\d5=241.18987833\d6=158.03994471\d7=33.18444321\d8=276.4498  
2607\d9=164.31501477\d10=44.1044687\d11=281.99899809\d12=166.53194298\d13=4  
7.87987524\d14=285.24437791\Version=EM64M-G09RevC.01\State=1-A\HF=-  
637.941526\RMSD=9.617e-09\RMSF=1.577e-04\Dipole=0.007359,-  
0.0002028,1.5287733\Quadrupole=3.1682288,2.0782061,-  
5.2464349,0.0572544,0.21069,-2.0311124\PG=C01 [X(B1H10N1Si2)]\@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1H10N1Si2\ROSMUSJ\18-Jun-  
2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6808936714\H,1,1.2075440252,2,106.04157348\H,1,1.  
2015227626,2,105.95381777,3,121.32457802,0\H,1,1.2091416632,2,104.24495926,3,24  
1.18987833,0\Si,2,1.7860156732,1,105.74623825,3,158.03994471,0\Si,2,1.7881740167,  
1,105.42640149,3,33.18444321,0\H,2,1.0177750256,1,107.30651279,3,276.44982607,0\  
H,6,1.4775945172,2,107.97297887,1,164.31501477,0\H,6,1.4663737687,2,109.1477416  
3,1,44.1044687,0\H,6,1.4699688027,2,105.8524078,1,281.99899809,0\H,7,1.479463671

2,2,107.89916974,1,166.53194298,0\H,7,1.466004078,2,107.36840081,1,47.87987524,0  
\H,7,1.4676737555,2,107.66869623,1,285.24437791,0\\Version=EM64M-  
G09RevC.01\State=1-A\HF=-662.9127814\RMSD=8.523e-09\Dipole=0.0079639,-  
0.0195893,1.581516\Quadrupole=3.1612358,2.2328926,-  
5.3941284,0.0471831,0.2242486,-2.1425152\PG=C01 [X(B1H10N1Si2)]\@

HF=-637.941526

Sum of electronic and zero-point Energies= -664.481786  
Sum of electronic and thermal Energies= -664.474251  
Sum of electronic and thermal Enthalpies= -664.473306  
Sum of electronic and thermal Free Energies= -664.512620  
NImag=0

H7N1Si2

-----  
0,1  
N  
Si,1,r2  
Si,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0

r2=1.72600649  
r3=1.72656253  
r4=1.01148513  
a3=128.51015237  
a4=115.79068565  
d4=186.56896575  
r5=1.47805173  
r6=1.47965513  
r7=1.47534888  
a5=110.97528746  
a6=112.51613634  
a7=107.02168195  
d5=55.33690958  
d6=-65.01131712  
d7=175.2832244  
r8=1.47741843  
r9=1.47547503

r10=1.48007382  
a8=109.70958434  
a9=107.69710496  
a10=113.18218915  
d8=143.91984203  
d9=23.88870161  
d10=-95.98356151

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H7N1Si2\ROSMUS\20-Feb-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(calcfc,z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\Si,1,r2\Si,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\|r2=1.72600649\r3=1.72656253\r4=1.01148513\|a3=128.51015237\|a4=115.79068565\|d4=186.56896575\r5=1.47805173\r6=1.47965513\r7=1.47534888\|a5=110.97528746\|a6=112.51613634\|a7=107.02168195\|d5=55.33690958\|d6=-65.01131712\|d7=175.2832244\r8=1.47741843\r9=1.47547503\r10=1.48007382\|a8=109.70958434\|a9=107.69710496\|a10=113.18218915\|d8=143.91984203\|d9=23.88870161\|d10=-95.98356151\|Version=IA64L-G09RevA.02\|State=1-A\|HF=-637.9489914\|RMSD=2.107e-09\|RMSF=3.497e-05\|Dipole=-0.3046689,0.0382738,-0.1411446\|Quadrupole=1.3545785,-1.1246274,-0.2299512,-0.3575325,1.0418542,-0.1217082\|PG=C01 [X(H7N1Si2)]\|@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\H7N1Si2\ROSMUSJ\20-Jun-2012\0\#\#p hf/cc-pvqz scf=verytight  
pop=(nboread,savenbos)\title\0,1\N\Si,1,1.72600649\Si,1,1.72656253,2,128.51015237\H,1,1.01148513,2,115.79068565,3,186.56896575,0\H,2,1.47805173,1,110.97528746,4,55.33690958,0\H,2,1.47965513,1,112.51613634,4,-65.01131712,0\H,2,1.47534888,1,107.02168195,4,175.2832244,0\H,3,1.47741843,1,109.70958434,2,143.91984203,0\H,3,1.47547503,1,107.69710496,2,23.88870161,0\H,3,1.48007382,1,113.18218915,2,-95.98356151,0\|Version=EM64M-G09RevC.01\|State=1-A\|HF=-636.4994612\|RMSD=9.769e-09\|Dipole=-0.3267659,0.0437177,-0.1508236\|Quadrupole=1.3825725,-1.0312194,-0.3513531,-0.3649255,1.1330354,-0.1284012\|PG=C01 [X(H7N1Si2)]\|@

HF=-637.9489914

Sum of electronic and zero-point Energies= -637.881960  
Sum of electronic and thermal Energies= -637.875792  
Sum of electronic and thermal Enthalpies= -637.874847  
Sum of electronic and thermal Free Energies= -637.912007  
NImag=0

H9N1Si3  
-----

--- Geometry Optimization ---

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H9N1Si3\ROSMUS\29-Jun-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread,savenbos) geom=allcheck  
guess=read\title\0,1\N\Si,1,1.73506631\Si,1,1.73539309,2,119.88663049\Si,1,1.735295  
17,2,120.06790565,3,178.0832973,0\H,2,1.47904633,1,107.28210627,4,179.83160549,0  
\H,2,1.47681702,1,111.28857518,5,119.5612662,0\H,2,1.47754083,1,111.46452017,5,24  
0.38737876,0\H,3,1.47729477,1,111.29975927,2,296.34330682,0\H,3,1.47784739,1,111.  
22216753,8,120.70282652,0\H,3,1.47868202,1,107.37725503,8,-  
119.67389413,0\H,4,1.47701059,1,111.13965551,2,124.47060507,0\H,4,1.47754878,1,1  
11.45031219,11,120.71999092,0\H,4,1.47871904,1,107.33868254,11,240.29206869,0\  
Version=IA64L-G09RevA.02\State=1-A\HF=-926.6372951\RMSD=2.497e-09\Dipole=-  
0.0014129,-0.0013254,-0.0024666\Quadrupole=0.2036362,-0.4039564,0.2003202,-  
0.0169858,-0.0047123,-0.0051648\PG=C01 [X(H9N1Si3)]\@
```

HF=-347.2470696

Sum of electronic and zero-point Energies=	-928.568348
Sum of electronic and thermal Energies=	-928.560191
Sum of electronic and thermal Enthalpies=	-928.559247
Sum of electronic and thermal Free Energies=	-928.601234

NImag=0

B1H12N1Si3

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
Si,2,r6,1,a6,3,d6,0  
Si,2,r7,1,a7,3,d7,0  
Si,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,6,r10,2,a10,1,d10,0  
H,6,r11,2,a11,1,d11,0  
H,7,r12,2,a12,1,d12,0  
H,7,r13,2,a13,1,d13,0  
H,7,r14,2,a14,1,d14,0  
H,8,r15,2,a15,1,d15,0  
H,8,r16,2,a16,1,d16,0

H,8,r17,2,a17,1,d17,0

r2=1.69529733  
r3=1.20701618  
r4=1.20676748  
r5=1.20675591  
r6=1.78538293  
r7=1.78520006  
r8=1.78554513  
r9=1.47909137  
r10=1.47164972  
r11=1.46720945  
r12=1.47959241  
r13=1.47093988  
r14=1.46704126  
r15=1.47899555  
r16=1.47188612  
r17=1.46669023  
a3=105.46754581  
a4=105.51818014  
a5=105.46005627  
a6=104.53847225  
a7=104.45322993  
a8=104.53266248  
a9=107.49158992  
a10=107.01205037  
a11=108.94290291  
a12=107.50828995  
a13=106.9820612  
a14=108.93740276  
a15=107.49959191  
a16=107.0227119  
a17=108.91174936  
d4=120.2003237  
d5=240.22858567  
d6=203.95191606  
d7=83.96418514  
d8=324.02121752  
d9=195.68486666  
d10=77.73158924  
d11=315.16636374  
d12=195.98597753  
d13=78.04171879  
d14=315.51040087  
d15=195.46196478  
d16=77.53723954

d17=314.9143943

--- Geometry Optimization ---

```
1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\B1H12N1Si3\ROSMUS\03-  
Mar-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Si,2,  
r6,1,a6,3,d6,0\Si,2,r7,1,a7,3,d7,0\Si,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d  
10,0\H,6,r11,2,a11,1,d11,0\H,7,r12,2,a12,1,d12,0\H,7,r13,2,a13,1,d13,0\H,7,r14,2,a14,1,  
d14,0\H,8,r15,2,a15,1,d15,0\H,8,r16,2,a16,1,d16,0\H,8,r17,2,a17,1,d17,0\r2=1.6952973  
3\r3=1.20701618\r4=1.20676748\r5=1.20675591\r6=1.78538293\r7=1.78520006\r8=1.7  
8554513\r9=1.47909137\r10=1.47164972\r11=1.46720945\r12=1.47959241\r13=1.4709  
3988\r14=1.46704126\r15=1.47899555\r16=1.47188612\r17=1.46669023\a3=105.46754  
581\a4=105.51818014\a5=105.46005627\a6=104.53847225\a7=104.45322993\a8=104.5  
3266248\a9=107.49158992\a10=107.01205037\a11=108.94290291\a12=107.50828995\a  
13=106.9820612\a14=108.93740276\a15=107.49959191\a16=107.0227119\a17=108.911  
74936\d4=120.2003237\d5=240.22858567\d6=203.95191606\d7=83.96418514\d8=324.0  
2121752\d9=195.68486666\d10=77.73158924\d11=315.16636374\d12=195.98597753\d  
13=78.04171879\d14=315.51040087\d15=195.46196478\d16=77.53723954\d17=314.91  
43943\Version=IA64L-G09RevA.02\State=1-A\HF=-928.6433529\RMSD=3.053e-  
09\RMSF=9.661e-05\Dipole=0.0003906,-  
0.0007575,1.2642507\Quadrupole=2.8301786,2.8261364,-5.6563149,0.0009539,-  
0.0028152,-0.0072159\PG=C01 [X(B1H12N1Si3)]\@
```

--- NBO Single Point ---

```
1\1\GINC-MH325M16MH\Freq\RHF\CC-pVQZ\B1H12N1Si3\ROSMUSJ\19-Jun-  
2012\1\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos)  
freq\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\Si,2,r6,1,a6,3,d  
6,0\Si,2,r7,1,a7,3,d7,0\Si,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,6,r10,2,a10,1,d10,0\H,6,r1  
1,2,a11,1,d11,0\H,7,r12,2,a12,1,d12,0\H,7,r13,2,a13,1,d13,0\H,7,r14,2,a14,1,d14,0\H,8,r  
15,2,a15,1,d15,0\H,8,r16,2,a16,1,d16,0\H,8,r17,2,a17,1,d17,0\r2=1.69529733\r3=1.2070  
1618\r4=1.20676748\r5=1.20675591\r6=1.78538293\r7=1.78520006\r8=1.78554513\r9=  
1.47909137\r10=1.47164972\r11=1.46720945\r12=1.47959241\r13=1.47093988\r14=1.4  
6704126\r15=1.47899555\r16=1.47188612\r17=1.46669023\a3=105.46754581\a4=105.5  
1818014\a5=105.46005627\a6=104.53847225\a7=104.45322993\a8=104.53266248\a9=1  
07.49158992\a10=107.01205037\a11=108.94290291\a12=107.50828995\a13=106.98206  
12\a14=108.93740276\a15=107.49959191\a16=107.0227119\a17=108.91174936\d4=120  
.2003237\d5=240.22858567\d6=203.95191606\d7=83.96418514\d8=324.02121752\d9=1  
95.68486666\d10=77.73158924\d11=315.16636374\d12=195.98597753\d13=78.041718  
79\d14=315.51040087\d15=195.46196478\d16=77.53723954\d17=314.9143943\Versio  
n=EM64M-G09RevC.01\State=1-A\HF=-953.0410509\RMSD=9.163e-  
09\RMSF=1.663e-03\ZeroPoint=0.1222439\Thermal=0.1310301\Dipole=0.000018,-  
0.0010922,1.3071004\DipoleDeriv=0.4419628,-0.0247364,-  
0.000271,0.0261004,0.4422335,0.000397,0.00006,0.0001735,0.8722706,-1.5243625,-  
0.0112257,-0.0000113,0.0103074,-1.5232393,0.0006215,-0.0000558,0.0004639,-  
1.5732201,-0.3936392,0.0248485,0.0650348,-0.0011137,-  
0.1223876,0.0242047,0.0382302,0.0061844,-0.2458322,-0.2007864,-0.1110591,-  
0.0115572,-0.1361742,-0.3146102,-0.0687428,-0.013607,-0.0364631,-0.2458064,-
```

0.1795538,0.1237678,-0.0534932,0.0987232,-0.3373529,0.0437964,-  
0.0248722,0.0295657,-0.2460417,1.6968781,0.2997751,-  
0.2680212,0.2894738,1.1602003,-0.0744903,-0.2841346,-  
0.0856564,1.2310327,1.0392104,0.0910935,0.0702342,0.0804532,1.8167629,0.2686023,  
0.0683398,0.2881743,1.2316636,1.5490949,-0.3745296,0.1987939,-  
0.3850499,1.3070171,-0.1943636,0.2164161,-0.2028451,1.2316093,-0.2913286,-  
0.0273286,0.0304931,-0.0214093,-0.2489336,-0.0089679,0.0561133,-0.0011621,-  
0.3150959,-0.2886802,-0.0155266,0.0181659,-0.030855,-  
0.2699158,0.0182187,0.0163124,0.0065541,-0.2194096,-0.2941352,-  
0.0263198,0.0249483,-0.0053637,-0.2262048,0.0004042,0.0055879,0.0039546,-  
0.2173482,-0.2385667,-0.0092347,-0.0233529,-0.0031961,-0.3017495,-0.0219899,-  
0.0295244,-0.0480278,-0.3150458,-0.2547134,0.010828,0.0067961,-0.0044561,-  
0.304195,-0.0247328,-0.0024048,-0.0173959,-0.219529,-0.2293681,-0.032221,-  
0.0125314,-0.0111564,-0.2907292,-0.0218711,0.0006911,-0.0065717,-0.2171952,-  
0.2805051,0.0276628,-0.0076445,0.033479,-0.2596233,0.0308255,-  
0.027117,0.0491258,-0.3152285,-0.2945568,0.0275142,-0.0246892,0.0123125,-  
0.2638548,0.006758,-0.0138311,0.0109195,-0.219346,-0.2569502,0.0266916,-  
0.0128946,0.0479248,-0.2634179,0.0213302,-0.0062039,0.0030063,-  
0.2174775\Polar=93.40609,0.0135452,93.4005858,0.0070298,-  
0.0055322,91.6593866\PolarDeriv=-4.0001318,-  
0.0080547,3.9883754,3.441426,0.5476745,-0.0015884,-0.0238733,3.9936909,-  
0.0395363,-0.5365201,3.4419721,-  
0.0224031,2.087984,0.0014651,2.0933328,0.0015137,0.00195,-  
1.2066152,1.2639745,3.0796474,-1.2735056,-  
2.2035982,0.1430678,0.001489,3.0721122,-1.2724436,-3.0811045,-0.1412545,-  
2.1975226,0.0018116,-3.3831547,0.0012801,-  
3.3747892,0.0013634,0.0039569,0.8149006,6.5137522,-0.1854353,1.018113,-2.5892,-  
0.3963947,3.9768562,0.0114584,0.4231127,0.224859,0.0029356,-0.8172446,-  
0.1338473,-1.9071025,-0.0012218,-0.6882209,1.961574,-0.0295577,-1.9487327,-  
1.4725502,-1.50472,-2.134539,-1.0926313,-0.8765733,-2.1241187,-2.1109883,-  
1.9929474,-4.5001742,-0.4675414,-2.3140766,-3.3679944,-0.9937284,-0.528534,-  
1.6018462,-1.0099362,-1.6842238,-1.9533717,-1.5522612,1.2399385,-2.3678602,-  
1.4277599,0.6577228,-1.8522595,1.6646533,-1.9163814,4.7694044,1.0709924,-  
1.9743618,3.5223147,-0.9933212,0.5289184,-1.6053271,-0.9518684,1.7145626,-  
1.9477034,-1.4797876,-2.2875617,-1.6573524,1.8227483,-0.4483643,0.5594592,-  
2.9685724,0.3953977,4.3334841,-0.3251512,1.1498389,-2.2121684,2.8734877,-  
0.3524931,1.6968735,2.5318381,-1.1868004,-3.6623033,1.7297794,-  
3.5059688,1.0569576,1.6252874,0.4249368,-2.2292506,-  
1.3860797,0.6117286,3.4455789,0.5516232,1.3106437,0.6036942,2.2696155,0.6919189,  
2.2646196,-2.3259436,-1.6241611,-3.6333797,-0.6565262,-  
3.102274,1.0607288,0.9945079,-0.1453103,1.6267574,-4.5389774,-  
0.5559125,1.1529993,-0.0224399,1.9952271,1.5700994,1.6989551,-  
0.3184989,2.8852458,-0.2479792,2.7677454,-3.6916871,-1.4287183,0.2646397,-  
0.1453863,1.7925463,-0.0235912,-1.4984544,0.7724978,-0.3349543,0.6032667,-  
0.2796384,1.2312605,1.1761948,2.9502915,0.1956804,1.9968281,-  
2.5839998,0.4663512,8.8188253,0.3039376,-1.2224817,0.0042915,-

0.2396413,0.0070297,0.1042013,-2.6652701,-1.2057501,-9.4236142,0.1659198,-  
0.2116512,-1.6697702,-0.5214265,-0.0261699,-0.6428757,-0.3053946,-1.2054754,-  
0.3520174,-6.6805265,1.2265944,-1.4951965,-2.0674811,0.4874777,-  
2.0594062,2.4514005,-1.336622,1.5311856,0.5104678,-0.8978762,1.3299473,-  
3.4916421,0.4109013,-1.4033785,-1.9149606,0.7988251,-  
2.718169,1.1820631,0.5578893,0.8375789,1.5149062,0.4562627,1.7938366,0.1392035,0  
.4861919,0.5505972,0.1952338,1.5238561,0.7191004,2.0762098,0.3214957,2.8845766,1  
.719911,2.0112047,8.7958406,-6.3736428,2.6778737,-4.2573209,-0.2767181,-  
0.1423867,-1.4950209,2.3528371,-2.3989811,3.3930426,0.0170238,-0.147198,0.74072,-  
0.5706157,0.0571782,-0.5556937,-0.8875236,0.8657783,-  
0.3366347,4.4064734,2.3397675,3.0644171,-1.6237738,-  
0.7726278,2.1850805,1.8663815,1.9328661,3.2138198,-0.7486585,-  
1.3569832,1.1291533,-2.2842263,-1.116226,-2.6347793,1.6526714,1.2694594,-  
2.7537548,-0.1772506,-0.2915413,-0.2094154,1.2429104,-0.0439129,-0.2542127,-  
0.3773662,0.3214833,-1.6515629,-0.2976395,1.7766556,-1.8712387,2.406504,-  
0.5143237,2.5377936,0.9007936,-  
2.4596562,8.8335018,8.0900974,1.7696098,2.2227168,-0.1598117,-  
0.1155196,1.3940221,3.5407675,1.5773963,2.7684704,0.0414721,-  
0.3137833,0.9263732,-0.6548247,-0.0424084,-0.5368915,1.197179,0.3400292,-  
0.3634306,0.3313176,-1.047923,0.2873974,-0.753717,0.2405087,-0.1273909,-  
1.8001847,1.2721249,-7.290716,0.2631751,-2.1987563,-2.4419868,-  
1.5630053,0.6910378,-3.3154678,0.2607618,-2.0499882,-  
2.6952686\HyperPolar=3.5540637,14.0699089,-3.6869285,-14.4509371,-2.86067,-  
0.0834041,-3.0002413,0.2124505,0.1013761,88.6209485\PG=C01  
[X(B1H12N1Si3)]\NImag=0\0.40830467,0.00056333,0.40871300,0.00016081,0.000167  
15,0.17940059,-0.05422265,-0.00188035,-0.00003164,0.38681328,0.00183684,-  
0.05423750,0.00002154,0.00013361,0.38691345,-0.00000085,-0.00000509,-  
0.02605837,-0.00003465,-0.00015387,0.23298553,-  
0.19271530,0.00068733,0.03884774,0.00498188,-0.00077643,0.00623041,0.21195359,-  
0.00031384,-0.04104231,0.00117697,-0.00035858,0.00319788,0.00078026,-  
0.00022838,0.03643958,0.03381830,0.00064189,-0.04467750,0.02559205,0.00040093,-  
0.02216716,-0.04814346,-0.00088653,0.05893886,-0.07962735,-0.06566842,-  
0.01857025,0.00413040,0.00084033,-0.00246770,-0.01024205,-0.01843516,-  
0.00629855,0.08088641,-0.06660892,-0.15438881,-  
0.03439448,0.00128224,0.00407147,-0.00573183,-  
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0.00138955,0.00111556,-0.08075154,-0.08449889,0.00010543,-  
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0.00004134,0.00001518,0.00020659,0.00012678,-  
0.00012500,0.00036137,0.00004101,0.00028152,0.00040305,0.00001143,0.00002100,0.  
00020785,0.00001625,-0.01129325,-  
0.00738249,0.00006055,0.00144848,0.00388779,0.00138411,0.08452206,0.08595585\\-  
0.00011211,-0.00025577,0.00577198,-0.00011692,0.00010195,-0.00835837,-  
0.00025235,0.00055972,0.00126228,0.00030274,0.00016921,0.00127812,0.00011245,-  
0.00042155,0.00127398,-  
0.00027338,0.00028143,0.00111372,0.00015857,0.00007791,0.00096018,-0.00008684,-  
0.00057712,0.00102604,0.00061168,0.00049422,0.00100866,0.00115416,-0.00122810,-  
0.00086412,-0.00026845,0.00127601,-0.00168146,0.00017340,-  
0.00075634,0.00117968,-0.00139221,-0.00053536,-0.00082573,0.00114408,-  
0.00045250,-0.00175535,-0.00069965,0.00030873,0.00097600,0.00057396,0.00167697,-  
0.00084849,-0.00102914,-0.00071941,-0.00151711\\@1\1\GINC-  
MH325M16MH\SP\RHF\CC-pVQZ\B1H12N1Si3\ROSMUSJ\19-Jun-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\\title\\0,1\B\N,1,1.69529733\H,1,1.20701618,2,105.46754581\H,1,1.2067  
6748,2,105.51818014,3,120.2003237,0\H,1,1.20675591,2,105.46005627,3,240.22858567  
,0\Si,2,1.78538293,1,104.53847225,3,203.95191606,0\Si,2,1.78520006,1,104.45322993,  
3,83.96418514,0\Si,2,1.78554513,1,104.53266248,3,324.02121752,0\H,6,1.47909137,2,  
107.49158992,1,195.68486666,0\H,6,1.47164972,2,107.01205037,1,77.73158924,0\H,6,  
1.46720945,2,108.94290291,1,315.16636374,0\H,7,1.47959241,2,107.50828995,1,195.9  
8597753,0\H,7,1.47093988,2,106.9820612,1,78.04171879,0\H,7,1.46704126,2,108.9374  
0276,1,315.51040087,0\H,8,1.47899555,2,107.49959191,1,195.46196478,0\H,8,1.47188

612,2,107.0227119,1,77.53723954,0\H,8,1.46669023,2,108.91174936,1,314.9143943,0\  
Version=EM64M-G09RevC.01\State=1-A\HF=-953.0410509\RMSD=2.411e-  
09\Dipole=0.000018,-0.0010922,1.3070993\Quadrupole=2.8845931,2.8825528,-  
5.7671459,-0.0020731,-0.0039348,-0.0035393\PG=C01 [X(B1H12N1Si3)]\@

HF=-953.0410509

Sum of electronic and zero-point Energies= -952.918807  
Sum of electronic and thermal Energies= -952.910021  
Sum of electronic and thermal Enthalpies= -952.909077  
Sum of electronic and thermal Free Energies= -952.951145  
NImag=0

B1H6N1S1

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0  
S,2,r6,1,a6,3,d6,0  
H,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0

r2=1.65744289  
r3=1.20452184  
r4=1.20233506  
r5=1.20242975  
r6=1.74358098  
r7=1.01558396  
r8=1.01557782  
a3=103.2689154  
a4=104.6443367  
a5=104.6611785  
a6=110.62331872  
a7=108.05786663  
a8=108.19212512  
d4=119.84181808  
d5=240.30592599  
d6=180.41273645  
d7=59.34778765  
d8=301.53719886  
r9=1.34193771

a9=97.20968945  
d9=181.20215853

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1H6N1S1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\S,2,r  
6,1,a6,3,d6,0\H,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\r2=1.65744289\r3  
=1.20452184\r4=1.20233506\r5=1.20242975\r6=1.74358098\r7=1.01558396\r8=1.01557  
782\ a3=103.2689154\ a4=104.6443367\ a5=104.6611785\ a6=110.62331872\ a7=108.0578  
6663\ a8=108.19212512\ d4=119.84181808\ d5=240.30592599\ d6=180.41273645\ d7=59.3  
4778765\ d8=301.53719886\ r9=1.34193771\ a9=97.20968945\ d9=181.20215853\ \Version  
=EM64M-G09RevC.01\State=1-A\HF=-454.7179337\RMSD=8.893e-09\RMSF=6.434e-  
05\Dipole=0.2860896,0.009432,2.0609701\Quadrupole=1.6991139,0.1630853,-  
1.8621993,0.0120524,2.5391634,0.0744445\PG=C01 [X(B1H6N1S1)]\ \@

--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1H6N1S1\ROSMUSJ\14-Jun-  
2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nbread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6574428895\H,1,1.2045218372,2,103.2689154\H,1,1.2  
023350577,2,104.6443367,3,119.84181808,0\H,1,1.2024297477,2,104.6611785,3,240.30  
592599,0\S,2,1.7435809823,1,110.62331872,3,180.41273645,0\H,2,1.0155839621,1,108  
.05786663,3,59.34778765,0\H,2,1.015577825,1,108.19212512,3,301.53719886,0\H,6,1.3  
419377074,2,97.20968945,1,181.20215853,0\ \Version=EM64M-G09RevC.01\State=1-  
A\HF=-480.1789389\RMSD=5.547e-  
09\Dipole=0.3001862,0.0101003,2.1548861\Quadrupole=1.6609284,0.2513756,-  
1.9123039,0.0096062,2.6662059,0.076105\PG=C01 [X(B1H6N1S1)]\ \@

HF=-454.7179337

Sum of electronic and zero-point Energies=	-481.287437
Sum of electronic and thermal Energies=	-481.282246
Sum of electronic and thermal Enthalpies=	-481.281301
Sum of electronic and thermal Free Energies=	-481.315169
NImag=0	

H3N1S1

-----

0,1  
N  
S,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0

r2=1.70647426  
r3=1.01011789  
r4=1.01011782  
r5=1.33990786  
a3=111.08313078  
a4=111.08354546  
a5=97.34401041  
d4=122.66294985  
d5=241.31912311

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1S1\ROSMUSJ\14-Jun-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\S,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\r2=1.70647426  
\r3=1.01011789\r4=1.01011782\r5=1.33990786\ a3=111.08313078\ a4=111.08354546\ a5  
=97.34401041\ d4=122.66294985\ d5=241.31912311\ \Version=EM64M-  
G09RevC.01\State=1-A\HF=-454.7197605\RMSD=2.923e-09\RMSF=2.354e-  
05\Dipole=0.0893564,-0.1633046,-0.3780554\Quadrupole=-0.3890559,-  
0.0179224,0.4069782,-0.2884322,-1.2197625,2.2311829\PG=C01 [X(H3N1S1)]\@\@  
--- NBO Single Point ---

1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\H3N1S1\ROSMUSJ\15-Jun-2012\0\#\#p  
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\S,1,1.7064742668\H,1,1.0101178898,2,111.08313008\H,1,1.  
010117816,2,111.08354476,3,122.662948,0\H,2,1.3399078551,1,97.34401014,4,241.319  
12163,0\ \Version=EM64M-G09RevC.01\State=1-A\HF=-453.7546926\RMSD=4.956e-  
09\Dipole=0.0867639,-0.1585432,-0.3762389\Quadrupole=-  
0.3792774,0.0389,0.3403774,-0.3251072,-1.2736426,2.3297766\PG=C01  
[X(H3N1S1)]\@\@

HF=-454.7197605

Sum of electronic and zero-point Energies=	-454.684251
Sum of electronic and thermal Energies=	-454.680869
Sum of electronic and thermal Enthalpies=	-454.679925
Sum of electronic and thermal Free Energies=	-454.707997
NImag=0	

B1H6N1S2

-----  
0,1  
B  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,1,r5,2,a5,3,d5,0



S,2,r6,1,a6,3,d6,0  
S,2,r7,1,a7,3,d7,0  
H,2,r8,1,a8,3,d8,0  
H,6,r9,2,a9,1,d9,0  
H,7,r10,2,a10,1,d10,0

r2=1.68147277  
r3=1.20183144  
r4=1.20077026  
r5=1.20105586  
r6=1.74149422  
r7=1.74557004  
r8=1.01631216  
a3=103.2696627  
a4=103.32723517  
a5=103.97615217  
a6=107.71781291  
a7=107.88099938  
a8=104.96249727  
d4=119.81828671  
d5=240.1472546  
d6=177.1129573  
d7=49.93198466  
d8=293.53612052  
r9=1.34323595  
r10=1.34234356  
a9=96.37366856  
a10=96.37364937  
d9=175.08215324  
d10=174.64822967

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1H6N1S2\ROSMUSJ\16-Jun-2012\1\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\S,2,r  
6,1,a6,3,d6,0\S,2,r7,1,a7,3,d7,0\H,2,r8,1,a8,3,d8,0\H,6,r9,2,a9,1,d9,0\H,7,r10,2,a10,1,d10  
,0\r2=1.68147277\r3=1.20183144\r4=1.20077026\r5=1.20105586\r6=1.74149422\r7=1.  
74557004\r8=1.01631216\a3=103.2696627\a4=103.32723517\a5=103.97615217\a6=107  
.71781291\a7=107.88099938\a8=104.96249727\d4=119.81828671\d5=240.1472546\d6=  
177.1129573\d7=49.93198466\d8=293.53612052\r9=1.34323595\r10=1.34234356\a9=9  
6.37366856\a10=96.37364937\d9=175.08215324\d10=174.64822967\Version=EM64M-  
G09RevC.01\State=1-A\HF=-852.8889234\RMSD=6.597e-09\RMSF=1.873e-  
04\Dipole=0.0470829,-0.1910678,2.0841868\Quadrupole=0.6877937,0.3657282,-  
1.0535219,0.3086337,0.2806423,-1.1693214\PG=C01 [X(B1H6N1S2)]\@  
--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\B1H6N1S2\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.6814727678\H,1,1.2018314428,2,103.2696627\H,1,1.2007702559,2,103.32723517,3,119.81828671,0\H,1,1.2010558572,2,103.97615217,3,240.1472546,0\S,2,1.7414942157,1,107.71781291,3,177.1129573,0\S,2,1.7455700358,1,107.88099938,3,49.93198466,0\H,2,1.0163121571,1,104.96249727,3,293.53612052,0\H,6,1.3432359499,2,96.37366856,1,175.08215324,0\H,7,1.3423435557,2,96.37364937,1,174.64822967,0\Version=EM64M-G09RevC.01\State=1-A\HF=-877.6976736\RMSD=5.708e-09\Dipole=0.0548365,-0.2101258,2.2024084\Quadrupole=0.6056808,0.452434,-1.0581149,0.2356586,0.3177911,-1.2449337\PG=C01 [X(B1H6N1S2)]\@

HF=-852.8889234

Sum of electronic and zero-point Energies=	-879.451928
Sum of electronic and thermal Energies=	-879.445973
Sum of electronic and thermal Enthalpies=	-879.445029
Sum of electronic and thermal Free Energies=	-879.481289

NImag=0

H3N1S2

-----  
0,1  
N  
S,1,r2  
S,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.6857  
r3=1.6858  
r4=1.0086  
r5=1.349  
r6=1.349  
a3=122.3154  
a4=114.8201  
a5=100.3593  
a6=100.3654  
d4=212.8884  
d5=284.5113  
d6=288.4165

--- Geometry Optimization ---

1\1\GINC-MH325M15MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1S2\ROSMUSJ\16-Jun-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\S,1,r2\S,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\r2=1.6857\r3=1.6858\r4=1.0086\r5=1.349\r6=1.349\a3=122.3154\a4=114.8201\a5=100.3593\a6=100.3654\d4=212.8884\d5=284.5113\d6=288.4165\Version=EM64M-G09RevC.01\State=1-A\HF=-852.8924219\RMSD=6.722e-09\RMSF=1.836e-04\Dipole=-0.1232747,0.790778,-0.0678065\Quadrupole=-0.0598841,0.9363162,-0.8764321,0.5200254,0.6447441,0.287082\PG=C01 [X(H3N1S2)]\@

--- NBO Single Point ---

1\1\GINC-MH325M15MH\SP\RHF\CC-pVQZ\H3N1S2\ROSMUSJ\18-Jun-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\S,1,1.6857\S,1,1.6858,2,122.3154\H,1,1.0086,2,114.8201,3,212.8884,0\H,2,1.349,1,100.3593,4,284.5113,0\H,3,1.349,1,100.3654,2,288.4165,0\Version=EM64M-G09RevC.01\State=1-A\HF=-851.2866127\RMSD=6.054e-09\Dipole=-0.1186814,0.8557016,-0.0652957\Quadrupole=-0.0498764,1.0253075,-0.9754312,0.5891952,0.7307984,0.3251918\PG=C01 [X(H3N1S2)]\@

HF=-852.8924219

Sum of electronic and zero-point Energies=	-852.857427
Sum of electronic and thermal Energies=	-852.852954
Sum of electronic and thermal Enthalpies=	-852.852010
Sum of electronic and thermal Free Energies=	-852.884624

NImag=0

B1H6N1S3

-----  
0,1

B

N,1,r2

H,1,r3,2,a3

H,1,r4,2,a4,3,d4,0

H,1,r5,2,a5,3,d5,0

S,2,r6,1,a6,3,d6,0

S,2,r7,1,a7,3,d7,0

S,2,r8,1,a8,3,d8,0

H,6,r9,2,a9,1,d9,0

H,7,r10,2,a10,1,d10,0

H,8,r11,2,a11,1,d11,0

r2=1.70014122

r3=1.19854236

r4=1.20169629

r5=1.20210358

r6=1.758987

r7=1.76878292  
r8=1.75706485  
a3=103.63489567  
a4=102.95624782  
a5=102.89840285  
a6=104.75852749  
a7=110.75138257  
a8=105.24853914  
d4=120.36854598  
d5=239.89408784  
d6=185.65030702  
d7=63.01306941  
d8=306.21767686  
r9=1.34332265  
r10=1.34123042  
r11=1.34366048  
a9=95.45901676  
a10=93.48216539  
a11=95.72431407  
d9=187.19485192  
d10=49.79159288  
d11=185.41585287

--- Geometry Optimization ---

1\1\GINC-MH325M16MH\FOpt\RM062X\6-  
311++G(3df,2p)\B1H6N1S3\ROSMUSJ\18-Jun-2012\1\#\#p m062x 6-311++G(3df,2p)  
opt=(z-matrix,noeigen) optcyc=100 freq  
counterpoise=2\title\0,1\B\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,1,r5,2,a5,3,d5,0\H,1,r6,1,a6,3,d6,0\H,1,r7,1,a7,3,d7,0\H,1,r8,1,a8,3,d8,0\H,1,r9,2,a9,1,d9,0\H,1,r10,2,a10,1,d10,0\H,1,r11,2,a11,1,d11,0\|r2=1.70014122\r3=1.19854236\r4=1.20169629\r5=1.20210358\r6=1.758987\r7=1.76878292\r8=1.75706485\a3=103.63489567\a4=102.95624782\a5=102.89840285\a6=104.75852749\a7=110.75138257\a8=105.24853914\d4=120.36854598\d5=239.89408784\d6=185.65030702\d7=63.01306941\d8=306.21767686\r9=1.34332265\r10=1.34123042\r11=1.34366048\a9=95.45901676\a10=93.48216539\a11=95.72431407\d9=187.19485192\d10=49.79159288\d11=185.41585287\|Version=EM64M-G09RevC.01\State=1-A\HF=-1251.0538835\RMSD=9.091e-09\RMSF=6.630e-05\Dipole=-0.1493569,0.2144561,1.7281338\Quadrupole=-0.0221012,2.4404057,-2.4183045,-0.9988152,-0.299233,-1.7184338\PG=C01 [X(B1H6N1S3)]\@

--- NBO Single Point ---

1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\B1H6N1S3\ROSMUSJ\18-Jun-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\B\N,1,1.7001412164\H,1,1.1985423584,2,103.63489567\H,1,1.2016962889,2,102.95624782,3,120.36854598,0\H,1,1.2021035834,2,102.89840285,3,239.89408784,0\H,1,1.7589870037,1,104.75852749,3,185.65030702,0\H,1,1.7687829231,1,110.75138257,3,63.01306941,0\H,1,1.7570648539,1,105.24853914,3,306.21767686,0\H,1,1.3433226489,2,95.45901676,1,187.19485192,0\H,1,1.3412304154,2,93.48216539,1,4

9.79159288,0\H,8,1.3436604765,2,95.72431407,1,185.41585287,0\Version=EM64M-G09RevC.01\State=1-A\HF=-1275.2113632\RMSD=5.006e-09\Dipole=-0.1695797,0.2494272,1.8372043\Quadrupole=-0.12682,2.5776625,-2.4508424,-1.0420465,-0.3775169,-1.8438227\PG=C01 [X(B1H6N1S3)]\@\

HF=-1251.0538835

Sum of electronic and zero-point Energies= -1277.616784  
Sum of electronic and thermal Energies= -1277.609325  
Sum of electronic and thermal Enthalpies= -1277.608381  
Sum of electronic and thermal Free Energies= -1277.648132  
NImag=0

H3N1S3

-----  
0,1  
N  
S,1,r2  
S,1,r3,2,a3  
S,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0  
H,4,r7,1,a7,3,d7,0

r2=1.70214775  
r3=1.70161731  
r4=1.70186173  
r5=1.34845751  
r6=1.34853161  
r7=1.34855577  
a3=118.80635312  
a4=118.74083579  
a5=98.78057333  
a6=98.80827973  
a7=98.75619305  
d4=202.16218817  
d5=281.30599596  
d6=280.80739358  
d7=281.05097746

--- Geometry Optimization ---

1\1\GINC-MH325M14MH\FOpt\RM062X\6-311++G(3df,2p)\H3N1S3\ROSMUSJ\17-Jun-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\S,1,r2\S,1,r3,2,a3\S,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\H,4,r7,1,a7,3,d7,0\r2=1.70214775\r3=1.70161731\r4=1.70186173\r5=1.34845751\r6=

1.34853161\r7=1.34855577\|a3=118.80635312\|a4=118.74083579\|a5=98.78057333\|a6=9  
 8.80827973\|a7=98.75619305\|d4=202.16218817\|d5=281.30599596\|d6=280.80739358\|d7  
 =281.05097746\|Version=EM64M-G09RevC.01\|State=1-A\|HF=-  
 1251.0615652\|RMSD=3.331e-09\|RMSF=8.038e-  
 05\|Dipole=0.1653263,0.8568578,0.0988685\|Quadrupole=-1.2283419,2.53169,-  
 1.3033481,0.7523017,0.0769483,0.443685\|PG=C01 [X(H3N1S3)]\|@  
 --- NBO Single Point ---  
 \1\GINC-MH325M13MH\Freq\RHF\CC-pVQZ\H3N1S3\ROSMUSJ\19-Jun-2012\1\|#p  
 hf/cc-pvqz scf=verytight pop=(nboread,savenbos)  
 freq\|title\|0,1\|N\|S,1,r2\|S,1,r3,2,a3\|S,1,r4,2,a4,3,d4,0\|H,2,r5,1,a5,4,d5,0\|H,3,r6,1,a6,2,d6,  
 0\|H,4,r7,1,a7,3,d7,0\|r2=1.7024461\|r3=1.70229912\|r4=1.70268329\|r5=1.34853097\|r6=1.  
 34846306\|r7=1.34858334\|a3=118.63974812\|a4=118.54411702\|a5=98.75286435\|a6=98.  
 72305236\|a7=98.76197222\|d4=203.52357481\|d5=282.21578386\|d6=282.13674402\|d7=  
 281.95641405\|Version=EM64M-G09RevC.01\|State=1-A\|HF=-  
 1248.8115099\|RMSD=2.994e-09\|RMSF=4.696e-  
 03\|ZeroPoint=0.0364359\|Thermal=0.041804\|Dipole=0.1944762,0.9378805,0.1166322\|D  
 ipoleDeriv=-0.6430249,0.0406356,0.0032013,0.0402421,-  
 0.4580954,0.0241491,0.0074412,0.0234641,-0.6494961,-0.1435244,0.0847765,-  
 0.0168219,0.084781,0.2569138,-0.0830158,-0.0026482,-  
 0.0124735,0.5360486,0.3721297,0.0311684,-0.2827857,-  
 0.0303724,0.2551771,0.1173191,-0.2983214,0.0837345,0.0223733,0.3543803,-  
 0.0726178,0.3053478,-0.0106515,0.2740877,-0.0076305,0.3049323,-  
 0.0442904,0.0200533,0.1047606,-0.0463824,-0.011633,-0.0462438,-0.1155425,-  
 0.0605906,0.0236171,0.1143716,-0.0549245,-0.0140407,0.0770786,0.0882985,-  
 0.076471,-0.1143785,-0.013886,0.0510321,-0.0975046,0.0627329,-0.0306806,-  
 0.1146588,-0.085607,0.0387156,-0.0981622,0.0236547,-0.0860532,-  
 0.0673017,0.0632124\|Polar=67.4019485,-2.5095356,55.9404548,-0.3177546,-  
 1.4744197,67.7477473\|PolarDeriv=-1.1175626,-0.9594929,0.2963658,6.1774521,-  
 1.239225,-0.4179299,-3.3225096,0.7901218,-0.9063189,-1.2374946,0.4655324,-  
 1.9516597,5.8861969,-1.2416762,0.174831,0.069773,0.4103763,-6.8051796,-  
 0.5865906,-1.4484441,-1.4155671,2.7780665,-0.2990671,-0.5622794,-0.56225,-  
 1.5995178,-9.4151182,-0.2909028,1.3372288,-2.7732986,2.748925,-  
 0.5855249,0.0311709,-0.6666991,-3.298078,16.4662787,11.9856363,-3.253486,-  
 0.6869748,-4.6908758,0.3744329,4.2889574,-2.5405289,0.3774976,-  
 9.3575037,0.7350648,-2.1279569,-0.8187062,-4.5816107,0.6491313,-  
 1.3386433,4.2517779,-1.5125128,-5.6991956,-12.9499387,1.1257618,-2.2666562,-  
 4.6793917,0.7473356,-4.2444085,1.3778481,-3.5310441,-7.7483141,0.3737951,-  
 2.0645241,0.9477099,-4.5384105,0.7461878,-1.313775,-4.4877142,0.3142499,-  
 5.6456106,0.491774,1.2090118,1.2987819,0.8787142,0.501502,0.6335853,0.5577063,1.  
 4282062,8.4229752,0.4940871,3.2691491,3.1494927,0.0560048,0.259655,1.2999918,0.3  
 610052,1.8215201,2.2492043,2.4887704,2.0202471,1.7956276,-0.4139868,-  
 0.1492084,0.1197353,3.0053469,3.5864486,8.3595311,-0.7819616,-  
 0.217766,0.7270572,0.229111,0.1039185,0.6009293,0.7145226,1.0343697,-0.2688707,-  
 0.3120888,1.3064023,0.9784228,-0.0499784,0.0642299,0.1823398,1.4843873,-  
 1.0517122,10.6447486,0.7074119,-  
 0.6616634,0.7194048,0.1997835,0.0683085,0.5454953,-0.2426654,1.2300749,-

0.2966267\HyperPolar=4.8880228,9.515821,12.5909259,75.0555968,-  
32.7687962,8.7350803,7.5621861,0.019391,-0.07132,35.6364429\PG=C01  
[X(H3N1S3)]\NImag=0\0.38181748,-0.05340454,0.13636080,-0.00698773,-  
0.03160288,0.38910449,-0.04213172,0.00037209,-0.00326054,0.06595208,0.00053298,-  
0.04145642,-0.01724120,0.04876523,0.30179520,0.00652135,0.03207673,-0.20228100,-  
0.00068848,-0.00266053,0.28926334,-0.16451003,0.02814422,0.07342064,-  
0.00442354,-0.00607351,0.01816826,0.23824840,-0.01508075,-  
0.04121876,0.00809137,-0.00260387,0.00059297,-  
0.00529385,0.02277902,0.30014437,0.06285637,-0.01530457,-  
0.08033983,0.02886764,0.00029117,-0.03019100,-0.09343627,0.04760007,0.11887141,-  
0.14950502,0.01874133,-0.06348452,-0.00059643,0.00646413,-0.01891403,-  
0.04245924,0.01350580,-0.00354543,0.23207832,0.06191776,-  
0.05611016,0.03703092,0.00319483,-0.00334489,0.00225975,0.00359916,-  
0.00335324,0.00156150,0.00862602,0.30687353,-0.06373336,0.01129468,-0.08002730,-  
0.02649693,0.01180178,-  
0.03021651,0.00406399,0.00007194,0.01171867,0.10397275,0.00390010,0.11786449,0.  
00028725,0.00122141,-0.00134912,-0.01814650,-0.05009136,-  
0.00468384,0.00060290,0.00254573,-0.00015074,-0.00026720,-  
0.00222493,0.00035803,0.01636641,0.00120285,0.00596572,-0.00572209,-0.05009237,-  
0.25864161,-0.02425225,-  
0.00012679,0.00053258,0.00039442,0.00047975,0.00145238,0.00028627,0.04890217,0.  
25120267,-0.00606184,-0.03047715,-0.02282544,0.00045189,0.00212712,-0.03223532,-  
0.00439235,-0.00133956,0.00184100,0.00347866,-  
0.00295894,0.00188826,0.00614409,0.03087515,0.04955858,-0.02075042,-  
0.02609463,0.00493041,-0.00032129,0.00007056,-0.00383614,-0.03135361,-  
0.02372349,0.00684519,0.00294409,-  
0.00366394,0.00171886,0.00071199,0.00060910,0.00026830,0.04784144,-  
0.00447991,0.00593275,0.00387092,0.00028303,0.00053921,-0.00030469,-0.04677792,-  
0.25722877,-0.03548763,0.00049506,0.00142912,0.00028648,-0.00032077,-  
0.00039608,0.00086811,0.05202870,0.24983713,0.01044127,0.01564793,-  
0.00176744,0.00030878,0.00289635,0.00283861,0.00107357,-0.04807512,-0.02051207,-  
0.00146286,-0.00049467,-0.00140064,-0.00056437,-0.00070780,0.00089388,-  
0.00976205,0.03120066,0.01955252,-0.00520753,0.03102012,-0.00326913,-  
0.00033258,0.00033197,0.00343289,0.00389512,0.00257756,-0.00143676,-0.04219451,-  
0.07144889,-0.01988336,0.00044516,-0.00097471,0.00011125,0.00092782,-  
0.00122818,-0.00003433,0.04246654,0.00931161,-  
0.00947393,0.00557296,0.00008108,0.00051554,-0.00182517,-  
0.00154417,0.00053086,0.00094505,-0.04831210,-0.24694674,-0.02764125,-  
0.00003226,-0.00011567,0.00090528,0.00077370,-0.00011336,-  
0.00046734,0.03972214,0.25560331,-0.00303606,0.01836526,-  
0.00186348,0.00081765,0.00278531,0.00282187,0.00110216,-0.00105486,-0.00138818,-  
0.02004457,-0.04129865,-0.01982697,0.00024595,-0.00087369,0.00087904,-  
0.00016457,-0.00043385,0.00039514,0.02107945,0.02251048,0.01898259\0.00024316,-  
0.00023269,0.00005474,-0.00160547,-0.00791041,0.00563013,0.00400118,-  
0.00792474,-0.00433854,-0.00699970,-0.00556949,-  
0.00408688,0.00140573,0.00740856,-

0.00059395,0.00019165,0.00734149,0.00176422,0.00276345,0.00688729,0.00157029\\  
@

HF=-1248.8115099

Sum of electronic and zero-point Energies= -1248.775074  
Sum of electronic and thermal Energies= -1248.769706  
Sum of electronic and thermal Enthalpies= -1248.768762  
Sum of electronic and thermal Free Energies= -1248.804560  
NImag=0

## Implicit Solvation

Br3N1

-----  
0,1  
N  
Br,1,r2  
Br,1,r3,2,a3  
Br,1,r4,2,a4,3,d4,0

r2=1.89977744  
r3=1.89943903  
r4=1.89943901  
a3=109.23585892  
a4=109.23585877  
d4=119.47998203

--- Geometry Optimization ---

1\1\GINC-POPLE\FOpt\RM062X\6-311++G(3df,2p)\Br3N1\ROSMUS\06-Jul-2012\1\#\#p m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen) scrf=(pcm,solvent=water) freq\title\0,1\N\Br,1,r2\Br,1,r3,2,a3\Br,1,r4,2,a4,3,d4,0\r2=1.89977744\r3=1.89943903\r4=1.89943901\a3=109.23585892\a4=109.23585877\d4=119.47998203\Version=IA64L-G09RevA.02\State=1-A\HF=-7777.1599851\RMSD=2.807e-09\RMSF=1.383e-04\Dipole=0.1300071,-0.2228376,0.0914901\Quadrupole=0.4246605,-1.2808391,0.8561786,1.5084626,-0.620685,1.0638748\PG=C01 [X(Br3N1)]\@

--- NBO Single Point ---

1\1\GINC-POPLE\SP\RHF\CC-pVTZ\Br3N1\ROSMUS\06-Jul-2012\0\#\#p hf/cc-pvtz pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck guess=read\title\0,1\N\Br,1,1.89977744\Br,1,1.89943903,2,109.23585892\Br,1,1.89943901,2,109.23585877,3,119.47998203,0\Version=IA64L-G09RevA.02\State=1-A\HF=-7771.7259989\RMSD=3.052e-09\Dipole=0.1664639,-0.285326,0.1186195\Quadrupole=0.4346515,-1.3088613,0.8742097,1.5420809,-0.6372623,1.0922926\PG=C01 [X(Br3N1)]\@



HF=-7777.1599851

Sum of electronic and zero-point Energies= -7777.154622  
Sum of electronic and thermal Energies= -7777.149540  
Sum of electronic and thermal Enthalpies= -7777.148596  
Sum of electronic and thermal Free Energies= -7777.186953  
NImag=0

C3H9N1

-----  
0,1  
N  
C,1,r2  
C,1,r3,2,a3  
C,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0  
H,4,r11,1,a11,3,d11,0  
H,4,r12,1,a12,3,d12,0  
H,4,r13,1,a13,3,d13,0

r2=1.45215134  
r3=1.45221321  
r4=1.45217537  
a3=110.43345048  
a4=110.37352041  
d4=122.35911908  
r5=1.10244016  
r6=1.08991824  
r7=1.08998446  
a5=111.81020307  
a6=109.93443873  
a7=109.90266193  
d5=60.995754  
d6=-59.28619913  
d7=181.23770935  
r8=1.08989246  
r9=1.1024545  
r10=1.08996529  
a8=109.90064854  
a9=111.86213703

a10=109.92858327  
d8=181.36689078  
d9=61.11248627  
d10=-59.1931571  
r11=1.10248278  
r12=1.08989153  
r13=1.08990068  
a11=111.81927346  
a12=109.94435732  
a13=109.91371657  
d11=61.06539951  
d12=-59.22554393  
d13=181.29555485

--- Geometry Optimization ---

1\1\GINC-POPLE\FOpt\RM062X\6-311++G(3df,2p)\C3H9N1\ROSMUS\06-Jul-2012\1\#p nosym m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen)  
scrf=(pcm,solvent=water)  
freq\title\0,1\N\C,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.45215134\r3=1.45221321\r4=1.45217537\a3=110.43345048\a4=110.37352041\d4=122.35911908\r5=1.10244016\r6=1.08991824\r7=1.08998446\a5=111.81020307\a6=109.93443873\a7=109.90266193\d5=60.995754\d6=-59.28619913\d7=181.23770935\r8=1.08989246\r9=1.1024545\r10=1.08996529\a8=109.90064854\a9=111.86213703\a10=109.92858327\d8=181.36689078\d9=61.11248627\d10=-59.1931571\r11=1.10248278\r12=1.08989153\r13=1.08990068\a11=111.81927346\a12=109.94435732\a13=109.91371657\d11=61.06539951\d12=-59.22554393\d13=181.29555485\\Version=IA64L-G09RevA.02\HF=-174.4427906\RMSD=2.469e-09\RMSF=4.946e-05\Dipole=0.1786448,-0.3246752,0.1240899\Quadrupole=0.3121901,-0.8932292,0.581039,0.9507579,-0.3640396,0.6601023\PG=C01 [X(C3H9N1)]\@

--- NBO Single Point ---

1\1\GINC-POPLE\SP\RHF\CC-pVTZ\C3H9N1\ROSMUS\06-Jul-2012\0\#p hf/cc-pvtz  
pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck  
guess=read\title\0,1\N\C,1,1.4521513434\C,1,1.4522132141,2,110.43345048\C,1,1.4521753732,2,110.37352041,3,122.35911908,0\H,2,1.1024401578,1,111.81020307,4,60.995754,0\H,2,1.0899182353,1,109.93443873,4,-59.28619913,0\H,2,1.0899844645,1,109.90266193,4,181.23770935,0\H,3,1.089892458,1,109.90064854,2,181.36689078,0\H,3,1.1024544968,1,111.86213703,2,61.11248627,0\H,3,1.0899652859,1,109.92858327,2,-59.1931571,0\H,4,1.102482784,1,111.81927346,3,61.06539951,0\H,4,1.0898915313,1,109.94435732,3,-59.22554393,0\H,4,1.089900683,1,109.91371657,3,181.29555485,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-173.3355345\RMSD=7.526e-09\Dipole=0.1714777,-

0.3118155,0.1193035\Quadrupole=0.3414701,-0.9754907,0.6340206,1.0373853,-  
0.397644,0.7206775\PG=C01 [X(C3H9N1)]\@

HF=-174.4427906

Sum of electronic and zero-point Energies= -174.321942  
Sum of electronic and thermal Energies= -174.316600  
Sum of electronic and thermal Enthalpies= -174.315656  
Sum of electronic and thermal Free Energies= -174.349136  
NImag=0

Cl3N1

-----  
0,1  
N  
Cl,1,r2  
Cl,1,r3,2,a3  
Cl,1,r4,2,a4,3,d4,0

r2=1.73699531  
r3=1.73754051  
r4=1.73754051  
a3=108.51059986  
a4=108.51059986  
d4=117.83994713

--- Geometry Optimization ---

1\1\GINC-POPLE\POpt\RM062X\6-311++G(3df,2p)\Cl3N1\ROSMUS\06-Jul-  
2012\1\#p m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen) scrf=(pcm,solvent=water)  
freq\title\0,1\N\Cl,1,r2\Cl,1,r3,2,a3\Cl,1,r4,2,a4,3,d4,0\r2=1.73699531\r3=1.73754051\  
r4=1.73754051\a3=108.51059986\a4=108.51059986\d4=117.83994713\Version=IA64L  
-G09RevA.02\State=1-A\HF=-1435.2281642\RMSD=6.481e-09\RMSF=1.507e-  
04\Dipole=0.0974556,-0.1616814,0.0696785\Quadrupole=0.2688105,-  
0.8422728,0.5734624,1.0519002,-0.4551447,0.7550971\PG=CS  
[SG(Cl1N1),X(Cl2)]\@

--- NBO Single Point ---

1\1\GINC-POPLE\SP\RHF\CC-pVTZ\Cl3N1\ROSMUS\06-Jul-2012\0\#p hf/cc-pvtz  
pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck  
guess=read\title\0,1\N\Cl,1,1.7369953071\Cl,1,1.7375405077,2,108.51059986\Cl,1,1.7  
375405077,2,108.51059986,3,117.83994713,0\Version=IA64L-G09RevA.02\State=1-  
A\HF=-1432.8770608\RMSD=8.050e-09\Dipole=0.1215343,-  
0.2016286,0.0876399\Quadrupole=0.2506755,-0.7776547,0.5269793,0.973555,-  
0.4205642,0.6977271\PG=CS [SG(Cl1N1),X(Cl2)]\@

HF=-1435.2281642

Sum of electronic and zero-point Energies= -1435.221435  
 Sum of electronic and thermal Energies= -1435.216974  
 Sum of electronic and thermal Enthalpies= -1435.216029  
 Sum of electronic and thermal Free Energies= -1435.250514  
 NImag=0

F3N1

-----  
 0,1  
 N  
 F,1,r2  
 F,1,r3,2,a3  
 F,1,r4,2,a4,3,d4,0

r2=1.35070106  
 r3=1.35094066  
 r4=1.35094066  
 a3=102.01806214  
 a4=102.01806214  
 d4=105.27979459

--- Geometry Optimization ---

1\1\GINC-POPLE\POpt\RM062X\6-311++G(3df,2p)\F3N1\ROSMUS\06-Jul-2012\1\#p  
 m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen) scrf=(pcm,solvent=water)  
 freq\title\0,1\N\F,1,r2\F,1,r3,2,a3\F,1,r4,2,a4,3,d4,0\r2=1.35070106\r3=1.35094066\r4=  
 1.35094066\a3=102.01806214\a4=102.01806214\d4=105.27979459\Version=IA64L-  
 G09RevA.02\State=1-A\HF=-354.0962677\RMSD=7.773e-09\RMSF=2.051e-  
 04\Dipole=-0.054177,0.0709629,-0.0432473\Quadrupole=-0.0009734,0.0024324,-  
 0.001459,-0.0062333,0.0027208,-0.0035638\PG=CS [SG(F1N1),X(F2)]\@

--- NBO Single Point ---

1\1\GINC-POPLE\SP\RHF\CC-pVTZ\F3N1\ROSMUS\06-Jul-2012\0\#p hf/cc-pvtz  
 pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck  
 guess=read\title\0,1\N\F,1,1.3507010609\F,1,1.3509406581,2,102.01806214\F,1,1.3509  
 406581,2,102.01806214,3,105.27979459,0\Version=IA64L-G09RevA.02\State=1-  
 A\HF=-352.6807952\RMSD=4.313e-09\Dipole=-0.0798133,0.1045423,-  
 0.0643382\Quadrupole=-0.013153,0.0610452,-0.0478922,-0.1357997,0.0835504,-  
 0.1094373\PG=CS [SG(F1N1),X(F2)]\@

HF=-354.0962677

Sum of electronic and zero-point Energies= -354.085133  
 Sum of electronic and thermal Energies= -354.081693  
 Sum of electronic and thermal Enthalpies= -354.080749  
 Sum of electronic and thermal Free Energies= -354.111157

NImag=0

Ge3H9N1

-----  
0,1

N

Ge,1,r2

Ge,1,r3,2,a3

Ge,1,r4,2,a4,3,d4,0

H,2,r5,1,a5,4,d5,0

H,2,r6,1,a6,4,d6,0

H,2,r7,1,a7,4,d7,0

H,3,r8,1,a8,2,d8,0

H,3,r9,1,a9,2,d9,0

H,3,r10,1,a10,2,d10,0

H,4,r11,1,a11,3,d11,0

H,4,r12,1,a12,3,d12,0

H,4,r13,1,a13,3,d13,0

r2=1.84768213

r3=1.84763775

r4=1.8473925

a3=119.8299439

a4=120.12392718

d4=179.96782728

r5=1.54596461

r6=1.54497101

r7=1.54590052

a5=110.32485955

a6=106.85998909

a7=110.31118351

d5=119.69693928

d6=-0.20705465

d7=239.8652925

r8=1.54591986

r9=1.54592765

r10=1.54507815

a8=110.35368853

a9=110.36775368

a10=106.81965915

d8=240.00816377

d9=119.74308879

d10=-0.12674859

r11=1.54581003

r12=1.54497003

r13=1.54588076  
a11=110.34844831  
a12=106.78245821  
a13=110.39584023  
d11=120.25278466  
d12=0.35100998  
d13=240.45656011

--- Geometry Optimization ---

```
1\1\GINC-POPLE\FOpt\RM062X\6-311++G(3df,2p)\Ge3H9N1\ROSMUS\09-Jul-2012\1\#p nosym m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen)
scrf=(pcm,solvent=water)
freq\title\0,1\N\Ge,1,r2\Ge,1,r3,2,a3\Ge,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.84768213\r3=1.84763775\r4=1.8473925\ a3=119.8299439\ a4=120.12392718\ d4=179.96782728\r5=1.54596461\r6=1.54497101\r7=1.54590052\ a5=110.32485955\ a6=106.85998909\ a7=110.31118351\ d5=119.69693928\ d6=-0.20705465\ d7=239.8652925\r8=1.54591986\r9=1.54592765\r10=1.54507815\ a8=110.35368853\ a9=110.36775368\ a10=106.81965915\ d8=240.00816377\ d9=119.74308879\ d10=-0.12674859\r11=1.54581003\r12=1.54497003\r13=1.54588076\ a11=110.34844831\ a12=106.78245821\ a13=110.39584023\ d11=120.25278466\ d12=0.35100998\ d13=240.45656011\ Version=IA64L-G09RevA.02\ HF=-6291.0795432\ RMSD=9.069e-09\ RMSF=3.639e-05\ Dipole=-0.000717,-0.000036,0.0003842\ Quadrupole=0.5647772,-1.1389076,0.5741303,0.0039033,-0.0030308,0.0035256\ PG=C01 [X(Ge3H9N1)]\ \@
--- NBO Single Point ---
1\1\GINC-POPLE\SP\RHF\CC-pVTZ\Ge3H9N1\ROSMUS\09-Jul-2012\0\#p hf/cc-pvtz
pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck
guess=read\title\0,1\N\Ge,1,1.8476821284\Ge,1,1.8476377479,2,119.8299439\Ge,1,1.8473924972,2,120.12392718,3,179.96782728,0\H,2,1.5459646111,1,110.32485955,4,119.69693928,0\H,2,1.5449710131,1,106.85998909,4,-0.20705465,0\H,2,1.5459005243,1,110.31118351,4,239.8652925,0\H,3,1.5459198565,1,110.35368853,2,240.00816377,0\H,3,1.5459276542,1,110.36775368,2,119.74308879,0\H,3,1.5450781453,1,106.81965915,2,-0.12674859,0\H,4,1.5458100271,1,110.34844831,3,120.25278466,0\H,4,1.5449700324,1,106.78245821,3,0.35100998,0\H,4,1.5458807639,1,110.39584023,3,240.45656011,0\ Version=IA64L-G09RevA.02\ State=1-A\ HF=-6285.9387793\ RMSD=2.162e-09\ Dipole=-0.0007919,-0.0000241,0.0002539\ Quadrupole=0.4646737,-0.9368938,0.4722201,0.0036003,-0.0017916,0.0034146\ PG=C01 [X(Ge3H9N1)]\ \@
```

HF=-6291.0795432

Sum of electronic and zero-point Energies=	-6291.003785
Sum of electronic and thermal Energies=	-6290.995315
Sum of electronic and thermal Enthalpies=	-6290.994370

Sum of electronic and thermal Free Energies= -6291.039413  
NImag=1

H3N1O3

-----  
0,1  
N  
O,1,r2  
O,1,r3,2,a3  
O,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0  
H,4,r7,1,a7,3,d7,0

r2=1.39099891  
r3=1.39107828  
r4=1.39115883  
r5=0.96338414  
r6=0.96339051  
r7=0.96351927  
a3=104.04835529  
a4=104.04601554  
a5=103.88016251  
a6=103.87555498  
a7=103.87590706  
d4=108.71011989  
d5=221.08989214  
d6=220.49885292  
d7=220.5423719

--- Geometry Optimization ---

1\1\GINC-POPLE\FOpt\RM062X\6-311++G(3df,2p)\H3N1O3\ROSMUS\06-Jul-2012\1\#p m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen) scrf=(pcm,solvent=water) freq\title\0,1\N\O,1,r2\O,1,r3,2,a3\O,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\H,4,r7,1,a7,3,d7,0\r2=1.39099891\r3=1.39107828\r4=1.39115883\r5=0.96338414\r6=0.96339051\r7=0.96351927\a3=104.04835529\a4=104.04601554\a5=103.88016251\a6=103.87555498\a7=103.87590706\d4=108.71011989\d5=221.08989214\d6=220.49885292\d7=220.5423719\Version=IA64L-G09RevA.02\State=1-A\HF=-282.092525\RMSD=4.892e-09\RMSF=1.865e-04\Dipole=-0.8769597,1.2116435,-0.6798152\Quadrupole=0.1712104,-0.6560167,0.4848063,1.1550096,-0.6765908,0.9054447\PG=C01 [X(H3N1O3)]\@

--- NBO Single Point ---

1\1\GINC-POPLE\SP\RHF\CC-pVTZ\H3N1O3\ROSMUS\06-Jul-2012\0\#p hf/cc-pvtz pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck guess=read\title\0,1\N\O,1,1.390998914\O,1,1.3910782751,2,104.04835529\O,1,1.3911

588344,2,104.04601554,3,108.71011989,0\H,2,0.9633841412,1,103.88016251,4,221.089  
89214,0\H,3,0.9633905145,1,103.87555498,2,220.49885292,0\H,4,0.9635192666,1,103.  
87590706,3,220.5423719,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-  
280.7393469\RMSD=3.682e-09\Dipole=-0.9017303,1.2461173,-  
0.699187\Quadrupole=0.161532,-0.6157346,0.4542026,1.0831633,-  
0.6361422,0.8488822\PG=C01 [X(H3N1O3)]\@

HF=-282.092525

Sum of electronic and zero-point Energies= -282.044094  
Sum of electronic and thermal Energies= -282.039040  
Sum of electronic and thermal Enthalpies= -282.038096  
Sum of electronic and thermal Free Energies= -282.071288  
NImag=0

H3N1Se3

-----  
0,1  
N  
X,1,1.  
Se,1,rS1,2,aS1  
Se,1,rS2,2,aS2,3,dS2,0  
Se,1,rS3,2,aS3,3,dS3,0  
H,3,rH1,1,aH1,2,dH1,0  
H,4,rH2,1,aH2,2,dH2,0  
H,5,rH3,1,aH3,2,dH3,0

rS1=1.85367103  
rS2=1.85391711  
rS3=1.85411781  
rH1=1.47715662  
rH2=1.47716806  
rH3=1.47710406  
aS1=94.18737366  
aS2=104.03059222  
aS3=98.30885953  
aH1=97.4404465  
aH2=97.5205837  
aH3=97.44377211  
dS2=119.99486197  
dS3=-118.73575162  
dH1=184.4428067  
dH2=181.97272236  
dH3=174.59177208



--- Geometry Optimization ---

```
1\1\GINC-POPLE\POpt\RM062X\6-311++G(3df,2p)\H3N1Se3\ROSMUS\09-Jul-2012\1\#p nosym m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen)
scrf=(pcm,solvent=water)
freq\title\0,1\N\X,1,1.\Se,1,rS1,2,aS1\Se,1,rS2,2,aS2,3,dS2,0\Se,1,rS3,2,aS3,3,dS3,0\H,3,rH1,1,aH1,2,dH1,0\H,4,rH2,1,aH2,2,dH2,0\H,5,rH3,1,aH3,2,dH3,0\rS1=1.85367103\rS2=1.85391711\rS3=1.85411781\rH1=1.47715662\rH2=1.47716806\rH3=1.47710406\aS1=94.18737366\aS2=104.03059222\aS3=98.30885953\aN1=97.4404465\aN2=97.5205837\aN3=97.44377211\dS2=119.99486197\dS3=-118.73575162\dH1=184.4428067\dH2=181.97272236\dH3=174.59177208\Version=IA64L-G09RevA.02\HF=-7261.1579906\RMSD=8.431e-09\RMSF=4.009e-05\Dipole=0.0812787,0.0659091,-1.0477274\Quadrupole=-1.8280326,-1.8694455,3.6974781,0.0491414,-0.4140788,-0.3810801\PG=C01 [X(H3N1Se3)]\@
```

--- NBO Single Point ---

```
1\1\GINC-POPLE\SP\RHF\CC-pVTZ\H3N1Se3\ROSMUS\09-Jul-2012\0\#p hf/cc-pvtz
pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck
guess=read\title\0,1\N\X,1,1.\Se,1,1.8536710311,2,94.18737366\Se,1,1.8539171126,2,104.03059222,3,119.99486197,0\Se,1,1.8541178087,2,98.30885953,3,-118.73575162,0\H,3,1.4771566238,1,97.4404465,2,184.4428067,0\H,4,1.4771680606,1,97.5205837,2,181.97272236,0\H,5,1.477104062,1,97.44377211,2,174.59177208,0\Version=IA64L-G09RevA.02\State=1-A\HF=-7255.8144613\RMSD=7.326e-09\Dipole=0.0884982,0.0715745,-1.1292238\Quadrupole=-1.5755551,-1.613302,3.188857,0.0496153,-0.3535612,-0.3337634\PG=C01 [X(H3N1Se3)]\@
```

Sum of electronic and zero-point Energies=	-7261.127513
Sum of electronic and thermal Energies=	-7261.121156
Sum of electronic and thermal Enthalpies=	-7261.120212
Sum of electronic and thermal Free Energies=	-7261.160722
NImag=0	

H9N1Si3

```
-----
0,1
N
Si,1,r2
Si,1,r3,2,a3
Si,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,2,r6,1,a6,5,d6,0
H,2,r7,1,a7,5,d7,0
H,3,r8,1,a8,2,d8,0
H,3,r9,1,a9,8,d9,0
H,3,r10,1,a10,8,d10,0
```

H,4,r11,1,a11,2,d11,0  
H,4,r12,1,a12,11,d12,0  
H,4,r13,1,a13,11,d13,0

r2=1.73506631  
r3=1.73539309  
r4=1.73529517  
a3=119.88663049  
a4=120.06790565  
d4=178.0832973  
r5=1.47904633  
r6=1.47681702  
r7=1.47754083  
a5=107.28210627  
a6=111.28857518  
a7=111.46452017  
d5=179.83160549  
d6=119.5612662  
d7=240.38737876  
r8=1.47729477  
r9=1.47784739  
r10=1.47868202  
a8=111.29975927  
a9=111.22216753  
a10=107.37725503  
d8=296.34330682  
d9=120.70282652  
d10=-119.67389413  
r11=1.47701059  
r12=1.47754878  
r13=1.47871904  
a11=111.13965551  
a12=111.45031219  
a13=107.33868254  
d11=124.47060507  
d12=120.71999092  
d13=240.29206869

--- Geometry Optimization ---

1\1\GINC-POPLE\FOpt\RM062X\6-311++G(3df,2p)\H9N1Si3\ROSMUS\09-Jul-  
2012\1\#\#p nosym m062x/6-311++G(3df,2p) opt=(z-matrix,noeigen)  
scrf=(pcm,solvent=water)  
freq\title\0,1\N\Si,1,r2\Si,1,r3,2,a3\Si,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,5,d  
6,0\H,2,r7,1,a7,5,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,8,d9,0\H,3,r10,1,a10,8,d10,0\H,4,r1  
1,1,a11,2,d11,0\H,4,r12,1,a12,11,d12,0\H,4,r13,1,a13,11,d13,0\r2=1.73506631\r3=1.735  
39309\r4=1.73529517\a3=119.88663049\a4=120.06790565\d4=178.0832973\r5=1.4790

```

4633\r6=1.47681702\r7=1.47754083\a5=107.28210627\a6=111.28857518\a7=111.46452
017\d5=179.83160549\d6=119.5612662\d7=240.38737876\r8=1.47729477\r9=1.477847
39\r10=1.47868202\a8=111.29975927\a9=111.22216753\a10=107.37725503\d8=296.34
330682\d9=120.70282652\d10=-
119.67389413\r11=1.47701059\r12=1.47754878\r13=1.47871904\a11=111.13965551\a1
2=111.45031219\a13=107.33868254\d11=124.47060507\d12=120.71999092\d13=240.2
9206869\\Version=IA64L-G09RevA.02\HF=-928.6532661\RMSD=6.698e-
09\RMSF=1.384e-04\Dipole=-0.003262,-0.0036592,-
0.0026412\Quadrupole=0.2819584,-0.5629569,0.2809985,-0.0190032,-0.0103823,-
0.0050055\PG=C01 [X(H9N1Si3)]\@
--- NBO Single Point ---
1\1\GINC-POPLE\SP\RHF\CC-pVTZ\H9N1Si3\ROSMUS\09-Jul-2012\0\#p hf/cc-pvtz
pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck
guess=read\title\0,1\N,Si,1,1.73506631\Si,1,1.73539309,2,119.88663049\Si,1,1.735295
17,2,120.06790565,3,178.0832973,0\H,2,1.47904633,1,107.28210627,4,179.83160549,0
\H,2,1.47681702,1,111.28857518,5,119.5612662,0\H,2,1.47754083,1,111.46452017,5,24
0.38737876,0\H,3,1.47729477,1,111.29975927,2,296.34330682,0\H,3,1.47784739,1,111.
22216753,8,120.70282652,0\H,3,1.47868202,1,107.37725503,8,-
119.67389413,0\H,4,1.47701059,1,111.13965551,2,124.47060507,0\H,4,1.47754878,1,1
11.45031219,11,120.71999092,0\H,4,1.47871904,1,107.33868254,11,240.29206869,0\\
Version=IA64L-G09RevA.02\State=1-A\HF=-926.6166928\RMSD=8.692e-09\Dipole=-
0.0020611,-0.0032627,-0.002628\Quadrupole=0.1802157,-0.3526715,0.1724558,-
0.0250927,-0.0072654,-0.0072698\PG=C01 [X(H9N1Si3)]\@

```

HF=-928.6532661

```

Sum of electronic and zero-point Energies=      -928.571249
Sum of electronic and thermal Energies=         -928.563548
Sum of electronic and thermal Enthalpies=       -928.562604
Sum of electronic and thermal Free Energies=    -928.604202
NImag=1

```

H3N1S3

```

-----
0,1
N
S,1,r2
S,1,r3,2,a3
S,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,3,r6,1,a6,2,d6,0
H,4,r7,1,a7,3,d7,0

```

r2=1.70558229

r3=1.70505081

r4=1.70565805  
r5=1.34692839  
r6=1.34745492  
r7=1.34697943  
a3=118.08036898  
a4=118.1399299  
a5=98.97663709  
a6=99.05019478  
a7=99.04055111  
d4=207.01413499  
d5=281.62532348  
d6=283.53726884  
d7=285.02514789

--- Geometry Optimization ---

1\1\GINC-POPLE\FOpt\RM062X\6-311++G(3df,2p)\H3N1S3\ROSMUS\09-Jul-2012\1\#p m062x/6-311++G(3df,2p) nosym opt=(z-matrix,noeigen)  
scrf=(pcm,solvent=water)  
freq\title\0,1\N\S,1,r2\S,1,r3,2,a3\S,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\H,4,r7,1,a7,3,d7,0\r2=1.70558229\r3=1.70505081\r4=1.70565805\r5=1.34692839\r6=1.34745492\r7=1.34697943\a3=118.08036898\a4=118.1399299\a5=98.97663709\a6=99.05019478\a7=99.04055111\d4=207.01413499\d5=281.62532348\d6=283.53726884\d7=285.02514789\Version=IA64L-G09RevA.02\HF=-1251.0681105\RMSD=4.594e-09\RMSF=1.421e-04\Dipole=0.3112265,1.2210414,0.1675754\Quadrupole=-1.7061498,3.652651,-1.9465012,1.5022152,0.2499983,0.7532242\PG=C01 [X(H3N1S3)]\@

--- NBO Single Point ---

1\1\GINC-POPLE\SP\RHF\CC-pVTZ\H3N1S3\ROSMUS\09-Jul-2012\0\#p hf/cc-pvtz  
pop=savenbos scf=verytight scrf=(pcm,solvent=water) geom=allcheck  
guess=read\title\0,1\N\S,1,1.7055822895\S,1,1.7050508133,2,118.08036898\S,1,1.7056580464,2,118.1399299,3,207.01413499,0\H,2,1.3469283863,1,98.97663709,4,281.62532348,0\H,3,1.3474549158,1,99.05019478,2,283.53726884,0\H,4,1.3469794334,1,99.04055111,3,285.02514789,0\Version=IA64L-G09RevA.02\State=1-A\HF=-1248.7995662\RMSD=4.165e-09\Dipole=0.3416223,1.3419037,0.1850186\Quadrupole=-1.417366,3.0252167,-1.6078507,1.2540189,0.2263284,0.6106152\PG=C01 [X(H3N1S3)]\@

HF=-1251.0681105

Sum of electronic and zero-point Energies=	-1251.033549
Sum of electronic and thermal Energies=	-1251.027788
Sum of electronic and thermal Enthalpies=	-1251.026844
Sum of electronic and thermal Free Energies=	-1251.063439
NImag=0	

## Carbon bound substituents

C4H11N1

0,1

N

C,1,r2

H,1,r3,2,a3

H,1,r4,2,a4,3,d4,0

H,2,r5,1,a5,4,d5,0

H,2,r6,1,a6,4,d6,0

C,2,r7,1,a7,4,d7,0

H,7,r8,2,a8,1,d8,0

H,7,r9,2,a9,1,d9,0

C,7,r10,2,a10,1,d10,0

H,10,r11,7,a11,2,d11,0

H,10,r12,7,a12,2,d12,0

C,10,r13,7,a13,2,d13,0

H,13,r14,10,a14,7,d14,0

H,13,r15,10,a15,7,d15,0

H,13,r16,10,a16,7,d16,0

r14=1.08968811

r15=1.09144751

r16=1.09184948

a14=111.2085363

a15=111.73621588

a16=110.8109612

d14=185.62753411

d15=65.47969725

d16=-54.31126438

r11=1.09186726

r12=1.09305566

r13=1.52626487

a11=108.55764962

a12=109.56273869

a13=113.44549019

d11=181.45741604

d12=66.45072237

d13=-56.77290215

r8=1.09392702

r9=1.09190883

r10=1.52946076

a8=108.36029236

a9=108.56727694

a10=113.93974266

d8=179.27732882

d9=62.89670484  
d10=-59.09096722  
r2=1.4619865  
r3=1.01317425  
r4=1.01201846  
a3=110.69046256  
a4=110.83905483  
d4=118.28778929  
r5=1.09774551  
r6=1.09109932  
r7=1.52360987  
a5=113.16619283  
a6=107.68420131  
a7=110.82252785  
d5=61.3949665  
d6=-56.26718198  
d7=184.8139438

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C4H11N1\ROSMUS\07-Aug-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\C,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\C,2,r7,1,a7,4,d7,0\H,7,r8,2,a8,1,d8,0\H,7,r9,2,a9,1,d9,0\C,7,r10,2,a10,1,d10,0\H,10,r11,7,a11,2,d11,0\H,10,r12,7,a12,2,d12,0\C,10,r13,7,a13,2,d13,0\H,13,r14,10,a14,7,d14,0\H,13,r15,10,a15,7,d15,0\H,13,r16,10,a16,7,d16,0\r14=1.08968811\r15=1.09144751\r16=1.09184948\ a14=111.2085363\ a15=111.73621588\ a16=110.8109612\ d14=185.62753411\ d15=65.47969725\ d16=-54.31126438\r11=1.09186726\r12=1.09305566\r13=1.52626487\ a11=108.55764962\ a12=109.56273869\ a13=113.44549019\ d11=181.45741604\ d12=66.45072237\ d13=-56.77290215\r8=1.09392702\r9=1.09190883\r10=1.52946076\ a8=108.36029236\ a9=108.56727694\ a10=113.93974266\ d8=179.27732882\ d9=62.89670484\ d10=-59.09096722\r2=1.4619865\r3=1.01317425\r4=1.01201846\ a3=110.69046256\ a4=110.83905483\ d4=118.28778929\r5=1.09774551\r6=1.09109932\r7=1.52360987\ a5=113.16619283\ a6=107.68420131\ a7=110.82252785\ d5=61.3949665\ d6=-56.26718198\ d7=184.8139438\ \Version=IA64L-G09RevA.02\State=1-A\HF=-213.7604577\RMSD=3.266e-09\RMSF=8.670e-05\Dipole=0.234609,-0.3574196,0.1647966\Quadrupole=-0.5096035,0.8505985,-0.340995,1.4617072,-1.3703917,1.692735\PG=C01 [X(C4H11N1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C4H11N1\ROSMUS\07-Aug-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\C,1,1.4619864963\H,1,1.0131742476,2,110.69046256\H,1,1.0120184552,2,110.83905483,3,118.28778929,0\H,2,1.0977455073,1,113.16619283,4,61.3949665,0\H,2,1.0910993243,1,107.68420131,4,-56.26718198,0\C,2,1.5236098736,1,110.82252785,4,184.8139438,0\H,7,1.0939270182,2,108.36029236,1,179.27732882,0\H,7,1.0919088304,2,108.56727694,1,62.89670484,0\C

,7,1.5294607597,2,113.93974266,1,-  
59.09096722,0\H,10,1.0918672627,7,108.55764962,2,181.45741604,0\H,10,1.09305566  
16,7,109.56273869,2,66.45072237,0\C,10,1.5262648672,7,113.44549019,2,-  
56.77290215,0\H,13,1.0896881142,10,111.2085363,7,185.62753411,0\H,13,1.09144750  
9,10,111.73621588,7,65.47969725,0\H,13,1.0918494799,10,110.8109612,7,-  
54.31126438,0\Version=IA64L-G09RevA.02\State=1-A\HF=-  
212.4109432\RMSD=6.994e-09\Dipole=0.2369547,-0.3762682,0.1548427\Quadrupole=-  
0.6507399,0.9217532,-0.2710133,1.421473,-1.4033302,1.6674257\PG=C01  
[X(C4H11N1)]\@

HF=-213.7604577

Sum of electronic and zero-point Energies= -213.610022  
Sum of electronic and thermal Energies= -213.603279  
Sum of electronic and thermal Enthalpies= -213.602335  
Sum of electronic and thermal Free Energies= -213.639905  
NImag=0

C1H4N2

-----  
0,1  
N  
C,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
N,2,r7,1,a7,4,d7,0

r2=1.37402431  
r3=1.00703658  
r4=1.00514817  
a3=118.38981702  
a4=118.42824982  
d4=148.22466624  
r5=1.89705242  
r6=1.08950984  
r7=1.26578174  
a5=98.55015399  
a6=112.89121774  
a7=128.51880966  
d5=162.25718995  
d6=-19.06595996  
d7=163.37220298

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C1H4N2\ROSMUS\08-Aug-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\C,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\N,2,r7,1,a7,4,d7,0\r2=1.37402431\r3=1.00703658\r4=1.00514817\a3=118.38981702\ a4=118.42824982\d4=148.22466624\r5=1.89705242\r6=1.08950984\r7=1.26578174\a5=98.55015399\a6=112.89121774\a7=128.51880966\d5=162.25718995\d6=-19.06595996\d7=163.37220298\Version=IA64L-G09RevA.02\State=1-A\HF=-149.9926577\RMSD=1.961e-09\RMSF=3.238e-05\Dipole=-0.257757,-0.3765334,-1.303795\Quadrupole=2.6943194,-1.1909982,-1.5033212,1.2750089,-1.4031966,0.6183169\PG=C01 [X(C1H4N2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C1H4N2\ROSMUS\08-Aug-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\C,1,1.3740243118\H,1,1.0070365776,2,118.38981702\H,1,1.0051481744,2,118.42824982,3,148.22466624,0\H,2,1.8970524201,1,98.55015399,4,162.25718995,0\H,2,1.0895098396,1,112.89121774,4,-19.06595996,0\N,2,1.2657817384,1,128.51880966,4,163.37220298,0\Version=IA64L-G09RevA.02\State=1-A\HF=-149.1503067\RMSD=6.055e-09\Dipole=-0.3085195,-0.406286,-1.3455594\Quadrupole=2.8163789,-1.1320013,-1.6843776,1.300441,-1.5168623,0.6240605\PG=C01 [X(C1H4N2)]\@

HF=-149.9926577

Sum of electronic and zero-point Energies=	-149.934454
Sum of electronic and thermal Energies=	-149.930634
Sum of electronic and thermal Enthalpies=	-149.929689
Sum of electronic and thermal Free Energies=	-149.958997
NImag=0	

C2H7N1

-----  
0,1  
N  
C,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
C,2,r7,1,a7,4,d7,0  
H,7,r8,2,a8,1,d8,0  
H,7,r9,2,a9,1,d9,0  
H,7,r10,2,a10,1,d10,0

r8=1.08984764



r9=1.08946329  
r10=1.09209326  
a8=111.09040074  
a9=110.25542655  
a10=110.63762514  
d8=178.13089079  
d9=57.30890237  
d10=-62.11362814  
r2=1.46184657  
r3=1.01351162  
r4=1.01232874  
a3=110.23128374  
a4=111.11548421  
d4=118.27857798  
r5=1.09724941  
r6=1.0914618  
r7=1.51892128  
a5=113.25933603  
a6=107.65275898  
a7=109.97186042  
d5=57.15025199  
d6=-60.84436703  
d7=179.88358637

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C2H7N1\ROSMUS\07-Aug-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\C,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\C,2,r7,1,a7,4,d7,0\H,7,r8,2,a8,1,d8,0\H,7,r9,2,a9,1,d9,0\H,7,r10,2,a10,1,d10,0\r8=1.08984764\r9=1.08946329\r10=1.09209326\a8=111.09040074\a9=110.25542655\a10=110.63762514\d8=178.13089079\d9=57.30890237\d10=-62.11362814\r2=1.46184657\r3=1.01351162\r4=1.01232874\a3=110.23128374\a4=111.11548421\d4=118.27857798\r5=1.09724941\r6=1.0914618\r7=1.51892128\a5=113.25933603\a6=107.65275898\a7=109.97186042\d5=57.15025199\d6=-60.84436703\d7=179.88358637\\Version=IA64L-G09RevA.02\State=1-A\HF=-135.1496046\RMSD=6.617e-09\RMSF=6.601e-05\Dipole=0.2307767,-0.4161884,0.1634994\Quadrupole=0.2563366,0.2331327,-0.4894693,0.5860394,-1.0942589,1.4900022\PG=C01 [X(C2H7N1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C2H7N1\ROSMUS\07-Aug-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read  
geom=allcheck\title\0,1\N\C,1,1.4618465716\H,1,1.0135116206,2,110.23128374\H,1,1.0123287404,2,111.11548421,3,118.27857798,0\H,2,1.0972494146,1,113.25933603,4,57.15025199,0\H,2,1.091461802,1,107.65275898,4,-60.84436703,0\C,2,1.5189212781,1,109.97186042,4,179.88358637,0\H,7,1.0898476355,2,111.09040074,1,178.13089079,0\H,7,1.0894632902,2,110.25542655,1,57.30890237,0\

H,7,1.0920932615,2,110.63762514,1,-62.11362814,0\\Version=IA64L-  
G09RevA.02\\State=1-A\\HF=-134.3141166\\RMSD=5.487e-09\\Dipole=0.2370302,-  
0.4329492,0.1528385\\Quadrupole=0.2673121,0.2427167,-0.5100288,0.5195683,-  
1.1152472,1.4492587\\PG=C01 [X(C2H7N1)]\\@

HF=-135.1496046

Sum of electronic and zero-point Energies= -135.056650  
Sum of electronic and thermal Energies= -135.052218  
Sum of electronic and thermal Enthalpies= -135.051274  
Sum of electronic and thermal Free Energies= -135.082168  
NImag=0

C1H5N1O1

-----  
0,1  
N  
C,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
O,2,r7,1,a7,4,d7,0  
H,7,r8,2,a8,1,d8,0

r8=0.9599954  
a8=109.57700868  
d8=179.99646965  
r2=1.42650013  
r3=1.01250746  
r4=1.0125247  
a3=110.51269263  
a4=110.51257932  
d4=119.07047627  
r5=1.09308944  
r6=1.0930804  
r7=1.42440042  
a5=108.6226865  
a6=108.62182107  
a7=110.80215466  
d7=59.48185514  
d6=-61.4208447  
d5=180.39741884

--- Geometry Optimization ---

```

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C1H5N1O1\ROSMUS\08-Aug-
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\N\C,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6
,0\O,2,r7,1,a7,4,d7,0\H,7,r8,2,a8,1,d8,0\r8=0.9599954\a8=109.57700868\d8=179.99646
965\r2=1.42650013\r3=1.01250746\r4=1.0125247\a3=110.51269263\a4=110.51257932\
d4=119.07047627\r5=1.09308944\r6=1.0930804\r7=1.42440042\a5=108.6226865\a6=10
8.62182107\a7=110.80215466\d7=59.48185514\d6=-
61.4208447\d5=180.39741884\Version=IA64L-G09RevA.02\State=1-A\HF=-
171.0723491\RMSD=4.972e-09\RMSF=2.578e-05\Dipole=-
0.025267,0.044071,0.4458577\Quadrupole=-0.3430819,-
2.1412523,2.4843341,1.6145334,-0.875915,1.4895634\PG=C01 [X(C1H5N1O1)]\@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C1H5N1O1\ROSMUS\08-Aug-2012\0\#p
hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\title\0,1\N\C,1,1.4265001315\H,1,1.0125074634,2,110.51269263\H,1,1,
0125247049,2,110.51257932,3,119.07047627,0\H,2,1.0930894414,1,108.6226865,4,180.
39741884,0\H,2,1.0930803982,1,108.62182107,4,-
61.4208447,0\O,2,1.4244004239,1,110.80215466,4,59.48185514,0\H,7,0.9599953962,2,
109.57700868,1,179.99646965,0\Version=IA64L-G09RevA.02\State=1-A\HF=-
170.1606445\RMSD=8.112e-09\Dipole=-0.0276215,0.0481288,0.4676048\Quadrupole=-
0.3203376,-2.1417619,2.4620995,1.6352554,-0.8977227,1.5266399\PG=C01
[X(C1H5N1O1)]\@

```

HF=-171.0723491

```

Sum of electronic and zero-point Energies=      -171.002082
Sum of electronic and thermal Energies=         -170.997972
Sum of electronic and thermal Enthalpies=       -170.997027
Sum of electronic and thermal Free Energies=    -171.027249
NImag=0

```

C3H9N1

```

-----
0,1
N
C,1,r2
H,1,r3,2,a3
H,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,2,r6,1,a6,4,d6,0
C,2,r7,1,a7,4,d7,0
H,7,r8,2,a8,1,d8,0
H,7,r9,2,a9,1,d9,0
C,7,r10,2,a10,1,d10,0
H,10,r11,7,a11,2,d11,0

```

H,10,r12,7,a12,2,d12,0  
H,10,r13,7,a13,2,d13,0

r11=1.08952298  
r12=1.09131179  
r13=1.09137476  
a11=111.43061078  
a12=111.04867638  
a13=110.84735583  
d11=180.96296732  
d12=60.72313347  
d13=-58.9501933  
r8=1.09436934  
r9=1.09157257  
r10=1.5239427  
a8=108.98681696  
a9=108.46286735  
a10=112.14858087  
d8=301.27972166  
d9=56.95992086  
d10=179.46571931  
r2=1.46128731  
r3=1.01346134  
r4=1.01224991  
a3=110.19737943  
a4=110.94614259  
d4=117.82639676  
r5=1.09898568  
r6=1.09276345  
r7=1.52036558  
a5=113.40831684  
a6=107.88087295  
a7=110.56946387  
d5=60.30465117  
d6=-57.76605852  
d7=183.11684235

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C3H9N1\ROSMUS\08-Aug-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\C,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\C,2,r7,1,a7,4,d7,0\H,7,r8,2,a8,1,d8,0\H,7,r9,2,a9,1,d9,0\C,7,r10,2,a10,1,d10,0\H,10,r11,7,a11,2,d11,0\H,10,r12,7,a12,2,d12,0\H,10,r13,7,a13,2,d13,0\r11=1.08952298\r12=1.09131179\r13=1.09137476\a11=111.43061078\a12=111.04867638\a13=110.84735583\d11=180.96296732\d12=60.72313347\d13=-58.9501933\r8=1.09436934\r9=1.09157257\r10=1.5239427\a8=108.98681696\a9=108.4

```

6286735\|a10=112.14858087\d8=301.27972166\d9=56.95992086\d10=179.46571931\r2=
1.46128731\r3=1.01346134\r4=1.01224991\|a3=110.19737943\|a4=110.94614259\d4=11
7.82639676\r5=1.09898568\r6=1.09276345\r7=1.52036558\|a5=113.40831684\|a6=107.8
8087295\|a7=110.56946387\d5=60.30465117\d6=-
57.76605852\d7=183.11684235\|Version=IA64L-G09RevA.02\|State=1-A\|HF=-
174.4552588\|RMSD=4.550e-09\|RMSF=1.224e-04\|Dipole=0.243505,-
0.3884028,0.1510312\|Quadrupole=0.3768751,0.7955119,-1.172387,0.5476072,-
1.3608256,1.9825168\|PG=C01 [X(C3H9N1)]\|@
--- NBO Single Point ---
1\|GINC-PAULING\|SP\|RHF\|CC-pVQZ\|C3H9N1\|ROSMUS\|08-Aug-2012\|0\|#p hf/cc-
pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\|title\|0,1\|N\|C,1,1.461287312\|H,1,1.0134613391,2,110.19737943\|H,1,1.0
122499057,2,110.94614259,3,117.82639676,0\|H,2,1.0989856841,1,113.40831684,4,60.3
0465117,0\|H,2,1.0927634542,1,107.88087295,4,-
57.76605852,0\|C,2,1.520365578,1,110.56946387,4,183.11684235,0\|H,7,1.0943693445,2
,108.98681696,1,301.27972166,0\|H,7,1.0915725713,2,108.46286735,1,56.95992086,0\|C
,7,1.5239426965,2,112.14858087,1,179.46571931,0\|H,10,1.0895229753,7,111.43061078
,2,180.96296732,0\|H,10,1.0913117883,7,111.04867638,2,60.72313347,0\|H,10,1.091374
765,7,110.84735583,2,-58.9501933,0\|Version=IA64L-G09RevA.02\|State=1-A\|HF=-
173.3642304\|RMSD=6.944e-09\|Dipole=0.2491949,-
0.4065829,0.1383071\|Quadrupole=0.4231616,0.8416028,-1.2647644,0.4810559,-
1.3971581,1.9420476\|PG=C01 [X(C3H9N1)]\|@

```

HF=-174.4552588

```

Sum of electronic and zero-point Energies=      -174.333516
Sum of electronic and thermal Energies=         -174.327845
Sum of electronic and thermal Enthalpies=       -174.326901
Sum of electronic and thermal Free Energies=     -174.361400
NImag=0

```

C6H6Br1N1

```

-----
0,1
N
H,1,r2
H,1,r3,2,a3
C,1,r8,2,a8,3,d8,0
C,4,r9,1,a9,3,d9,0
C,4,r10,1,a10,5,d10,0
C,5,r11,4,a11,1,d11,0
C,6,r12,4,a12,1,d12,0
C,7,r13,5,a13,1,d13,0
H,5,r14,4,a14,9,d14,0
H,6,r15,4,a15,9,d15,0

```

H,7,r16,5,a16,9,d16,0  
H,8,r17,6,a17,9,d17,0  
Br,9,r18,7,a18,8,d18,0

r2=1.00756863  
r3=1.00756853  
r8=1.39157686  
r9=1.39523923  
r10=1.39525857  
r11=1.38470703  
r12=1.38469391  
r13=1.38504053  
r14=1.08309131  
r15=1.08309135  
r16=1.08090601  
r17=1.08090591  
r18=1.89477642  
a3=112.03021818  
a8=115.28999902  
a9=120.71959446  
a10=120.71791487  
a11=120.87318435  
a12=120.87396879  
a13=119.66002936  
a14=119.52583836  
a15=119.52499579  
a16=120.20720555  
a17=120.20860721  
a18=119.78447773  
d8=134.50069863  
d9=-24.93401169  
d10=-177.09350489  
d11=-177.36565968  
d12=177.3620602  
d13=-2.53111955  
d14=179.70546714  
d15=-179.70348802  
d16=-179.98229272  
d17=179.97919088  
d18=-179.92775952

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C6H6Br1N1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\titl\0,1\N\H,1,r2\H,1,r3,2,a3\C,1,r8,2,a8,3,d8,0\C,4,r9,1,a9,3,d9,0\C,4,r10,1,a10,5,d10,0\C,5,r11,4,a11,1,d11,0\C,6,r12,4,a12,1,d12,0\C,7,r13,5,a13,1,d13,0\H,5,r14,4,a14,9,

d14,0\H,6,r15,4,a15,9,d15,0\H,7,r16,5,a16,9,d16,0\H,8,r17,6,a17,9,d17,0\Br,9,r18,7,a18,  
8,d18,0\r2=1.00756863\r3=1.00756853\r8=1.39157686\r9=1.39523923\r10=1.39525857  
\r11=1.38470703\r12=1.38469391\r13=1.38504053\r14=1.08309131\r15=1.08309135\r1  
6=1.08090601\r17=1.08090591\r18=1.89477642\a3=112.03021818\a8=115.28999902\a9  
=120.71959446\a10=120.71791487\a11=120.87318435\a12=120.87396879\a13=119.660  
02936\a14=119.52583836\a15=119.52499579\a16=120.20720555\a17=120.20860721\a1  
8=119.78447773\d8=134.50069863\d9=-24.93401169\d10=-177.09350489\d11=-  
177.36565968\d12=177.3620602\d13=-2.53111955\d14=179.70546714\d15=-  
179.70348802\d16=-179.98229272\d17=179.97919088\d18=-  
179.92775952\\Version=IA64L-G09RevA.02\State=1-A\HF=-  
2861.1498204\RMSD=4.424e-09\RMSF=4.839e-  
05\Dipole=1.0257285,0.4965133,0.6914424\Quadrupole=3.0530957,-  
5.6522724,2.5991767,3.4478622,0.5574851,2.3261421\PG=C01 [X(C6H6Br1N1)]\\@  
--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C6H6Br1N1\ROSMUS\20-Jul-2012\0\#p  
hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\\title\0,1\N\H,1,1.0075686321\H,1,1.007568533,2,112.03021818\C,1,1.3915  
768633,2,115.28999902,3,134.50069863,0\C,4,1.3952392301,1,120.71959446,3,-  
24.93401169,0\C,4,1.3952585737,1,120.71791487,5,-  
177.09350489,0\C,5,1.38470703,4,120.87318435,1,-  
177.36565968,0\C,6,1.3846939079,4,120.87396879,1,177.3620602,0\C,7,1.3850405277,  
5,119.66002936,1,-  
2.53111955,0\H,5,1.0830913072,4,119.52583836,9,179.70546714,0\H,6,1.0830913494,4  
,119.52499579,9,-179.70348802,0\H,7,1.0809060098,5,120.20720555,9,-  
179.98229272,0\H,8,1.0809059057,6,120.20860721,9,179.97919088,0\Br,9,1.89477641  
71,7,119.78447773,8,-179.92775952,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-  
2857.731534\RMSD=2.402e-  
09\Dipole=1.0583107,0.5026234,0.7134056\Quadrupole=3.0953917,-  
5.9275224,2.8321307,3.1846046,0.321778,2.1487874\PG=C01 [X(C6H6Br1N1)]\\@

HF=-2861.1498204

Sum of electronic and zero-point Energies= -2861.042132  
Sum of electronic and thermal Energies= -2861.035012  
Sum of electronic and thermal Enthalpies= -2861.034067  
Sum of electronic and thermal Free Energies= -2861.074547  
NImag=0

C8H11N1

-----  
0,1  
N  
H,1,r2  
H,1,r3,2,a3  
C,1,r8,2,a8,3,d8,0

C,4,r9,1,a9,3,d9,0  
C,4,r10,1,a10,5,d10,0  
C,5,r11,4,a11,1,d11,0  
C,6,r12,4,a12,1,d12,0  
C,7,r13,5,a13,1,d13,0  
H,5,r14,4,a14,9,d14,0  
H,6,r15,4,a15,9,d15,0  
H,7,r16,5,a16,9,d16,0  
H,8,r17,6,a17,9,d17,0  
C,9,r18,7,a18,8,d18,0  
H,14,r19,9,a19,7,d19,0  
H,14,r20,9,a20,7,d20,0  
C,14,r21,9,a21,7,d21,0  
H,17,r22,14,a22,16,d22,0  
H,17,r23,14,a23,16,d23,0  
H,17,r24,14,a24,16,d24,0

r22=1.09081719  
r23=1.09074435  
r24=1.08931694  
a22=111.23326428  
a23=111.26695491  
a24=110.51045773  
d22=182.79388497  
d23=62.41206181  
d24=302.60515066  
r2=1.00806253  
r3=1.00822369  
r8=1.39719206  
r9=1.3907578  
r10=1.39643448  
r11=1.38887433  
r12=1.38242693  
r13=1.38914015  
r14=1.08358875  
r15=1.08355658  
r16=1.08192335  
r17=1.08453106  
r18=1.51334091  
r19=1.09351522  
r20=1.09343207  
r21=1.52321882  
a3=111.19116512  
a8=114.97022466  
a9=120.88850635  
a10=120.84253544



a11=120.75074144  
a12=120.39110281  
a13=121.54181114  
a14=119.42973545  
a15=119.47497866  
a16=118.37522122  
a17=119.00095191  
a18=123.35377764  
a19=108.52946981  
a20=108.54667194  
a21=115.3437217  
d8=131.90876931  
d9=-25.07120355  
d10=-177.02750089  
d11=-177.23605387  
d12=177.32712795  
d13=-2.74920585  
d14=179.76676  
d15=-179.66392198  
d16=-179.91422914  
d17=180.04514986  
d18=180.03048217  
d19=122.87487572  
d20=-122.64869766  
d21=0.1373714

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C8H11N1\ROSMUS\24-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\H,1,r2\H,1,r3,2,a3\C,1,r8,2,a8,3,d8,0\C,4,r9,1,a9,3,d9,0\C,4,r10,1,a10,5,d10,0\C,5,r11,4,a11,1,d11,0\C,6,r12,4,a12,1,d12,0\C,7,r13,5,a13,1,d13,0\H,5,r14,4,a14,9,d14,0\H,6,r15,4,a15,9,d15,0\H,7,r16,5,a16,9,d16,0\H,8,r17,6,a17,9,d17,0\C,9,r18,7,a18,8,d18,0\H,14,r19,9,a19,7,d19,0\H,14,r20,9,a20,7,d20,0\C,14,r21,9,a21,7,d21,0\H,17,r22,14,a22,16,d22,0\H,17,r23,14,a23,16,d23,0\H,17,r24,14,a24,16,d24,0\r22=1.09081719\r23=1.09074435\r24=1.08931694\ a22=111.23326428\ a23=111.26695491\ a24=110.51045773\d22=182.79388497\d23=62.41206181\d24=302.60515066\r2=1.00806253\r3=1.00822369\r8=1.39719206\r9=1.3907578\r10=1.39643448\r11=1.38887433\r12=1.38242693\r13=1.38914015\r14=1.08358875\r15=1.08355658\r16=1.08192335\r17=1.08453106\r18=1.51334091\r19=1.09351522\r20=1.09343207\r21=1.52321882\ a3=111.19116512\ a8=114.97022466\ a9=120.88850635\ a10=120.84253544\ a11=120.75074144\ a12=120.39110281\ a13=121.54181114\ a14=119.42973545\ a15=119.47497866\ a16=118.37522122\ a17=119.00095191\ a18=123.35377764\ a19=108.52946981\ a20=108.54667194\ a21=115.3437217\ d8=131.90876931\ d9=-25.07120355\ d10=-177.02750089\ d11=-177.23605387\ d12=177.32712795\ d13=-2.74920585\ d14=179.76676\ d15=-179.66392198\ d16=-179.91422914\ d17=180.04514986\ d18=180.03048217\ d19=122.87487572\ d20=-

122.64869766\d21=0.1373714\\Version=IA64L-G09RevA.02\State=1-A\HF=-  
366.1861505\RMSD=2.745e-09\RMSF=1.374e-04\Dipole=0.3481178,-  
0.132202,0.2757805\Quadrupole=2.6404877,-  
4.5776239,1.9371362,3.5356334,0.9217238,2.3456106\PG=C01 [X(C8H11N1)]\\@  
--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C8H11N1\ROSMUS\24-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) guess=read  
geom=allcheck\\title\\0,1\N\H,1,1.008062534\H,1,1.0082236947,2,111.19116512\C,1,1.3  
971920553,2,114.97022466,3,131.90876931,0\C,4,1.3907577992,1,120.88850635,3,-  
25.07120355,0\C,4,1.3964344774,1,120.84253544,5,-  
177.02750089,0\C,5,1.3888743301,4,120.75074144,1,-  
177.23605387,0\C,6,1.3824269283,4,120.39110281,1,177.32712795,0\C,7,1.389140152  
2,5,121.54181114,1,-  
2.74920585,0\H,5,1.083588746,4,119.42973545,9,179.76676,0\H,6,1.0835565773,4,119.  
47497866,9,-179.66392198,0\H,7,1.0819233532,5,118.37522122,9,-  
179.91422914,0\H,8,1.0845310647,6,119.00095191,9,180.04514986,0\C,9,1.513340908  
2,7,123.35377764,8,180.03048217,0\H,14,1.0935152203,9,108.52946981,7,122.8748757  
2,0\H,14,1.0934320705,9,108.54667194,7,-  
122.64869766,0\C,14,1.5232188179,9,115.3437217,7,0.1373714,0\H,17,1.0908171863,1  
4,111.23326428,16,182.79388497,0\H,17,1.0907443496,14,111.26695491,16,62.412061  
81,0\H,17,1.0893169402,14,110.51045773,16,302.60515066,0\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-363.9500513\RMSD=5.583e-09\Dipole=0.3388307,-  
0.1661869,0.2712556\Quadrupole=2.7321903,-  
4.8246079,2.0924176,3.3707202,0.75484,2.1963438\PG=C01 [X(C8H11N1)]\\@

HF=-366.1861505

Sum of electronic and zero-point Energies=	-366.011778
Sum of electronic and thermal Energies=	-366.003177
Sum of electronic and thermal Enthalpies=	-366.002233
Sum of electronic and thermal Free Energies=	-366.045030
NImag=0	

C7H9N1

-----  
0,1  
N,0.0049738716,-0.038396942,-0.0013581423  
H,-0.0350192695,0.0909185539,1.0029298048  
H,0.9489441643,0.087087285,-0.3478920062  
C,-0.6535561267,-1.1834213129,-0.4781276008  
C,-0.3000786343,-1.7606237754,-1.7075059104  
C,-1.7261709566,-1.7461266693,0.234345221  
C,-1.0000664826,-2.8626044806,-2.2020891265  
C,-2.4154388576,-2.8467411772,-0.2726855954  
C,-2.0722501386,-3.4305318815,-1.5014972698

H,0.5255268823,-1.3430641751,-2.2810479513  
H,-2.0222342842,-1.3153951235,1.1892374728  
H,-0.6989486495,-3.2898639603,-3.1568861866  
H,-3.2394171529,-3.261797596,0.3054035186  
C,-2.8443888607,-4.6083346071,-2.0531032032  
H,-3.0499113494,-5.3559841412,-1.2771269556  
H,-3.813622204,-4.2984760193,-2.4679656549  
H,-2.2903211261,-5.1066883058,-2.8564390177

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RB3LYP\6-31+G(d)\C7H9N1\ROSMUS\03-Jan-2012\0\#p  
b3lyp 6-31+G\* opt=(noeigen) freq\4-methylalanine\0,1\N,0.0049738716,-  
0.038396942,-0.0013581423\H,-  
0.0350192695,0.0909185539,1.0029298048\H,0.9489441643,0.087087285,-  
0.3478920062\C,-0.6535561267,-1.1834213129,-0.4781276008\C,-0.3000786343,-  
1.7606237754,-1.7075059104\C,-1.7261709566,-1.7461266693,0.234345221\C,-  
1.0000664826,-2.8626044806,-2.2020891265\C,-2.4154388576,-2.8467411772,-  
0.2726855954\C,-2.0722501386,-3.4305318815,-1.5014972698\H,0.5255268823,-  
1.3430641751,-2.2810479513\H,-2.0222342842,-1.3153951235,1.1892374728\H,-  
0.6989486495,-3.2898639603,-3.1568861866\H,-3.2394171529,-  
3.261797596,0.3054035186\C,-2.8443888607,-4.6083346071,-2.0531032032\H,-  
3.0499113494,-5.3559841412,-1.2771269556\H,-3.813622204,-4.2984760193,-  
2.4679656549\H,-2.2903211261,-5.1066883058,-2.8564390177\Version=IA64L-  
G09RevA.02\State=1-A\HF=-326.933578\RMSD=9.540e-09\RMSF=8.466e-  
06\Dipole=0.4208724,0.0082204,0.3237632\Quadrupole=1.319159,-  
2.7365789,1.4174199,4.252491,-0.3372624,3.0972436\PG=C01 [X(C7H9N1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RB3LYP\Aug-CC-pVDZ\C7H9N1\ROSMUS\03-Jan-  
2012\0\#p b3lyp aug-cc-pvdz geom=allcheck guess=read scf=verytight  
pop=savenbos\4-methylalanine\0,1\N,0.0049738716,-0.038396942,-  
0.0013581423\H,0,-  
0.0350192695,0.0909185539,1.0029298048\H,0,0.9489441643,0.087087285,-  
0.3478920062\C,0,-0.6535561267,-1.1834213129,-0.4781276008\C,0,-0.3000786343,-  
1.7606237754,-1.7075059104\C,0,-1.7261709566,-1.7461266693,0.234345221\C,0,-  
1.0000664826,-2.8626044806,-2.2020891265\C,0,-2.4154388576,-2.8467411772,-  
0.2726855954\C,0,-2.0722501386,-3.4305318815,-1.5014972698\H,0,0.5255268823,-  
1.3430641751,-2.2810479513\H,0,-2.0222342842,-1.3153951235,1.1892374728\H,0,-  
0.6989486495,-3.2898639603,-3.1568861866\H,0,-3.2394171529,-  
3.261797596,0.3054035186\C,0,-2.8443888607,-4.6083346071,-2.0531032032\H,0,-  
3.0499113494,-5.3559841412,-1.2771269556\H,0,-3.813622204,-4.2984760193,-  
2.4679656549\H,0,-2.2903211261,-5.1066883058,-2.8564390177\Version=IA64L-  
G09RevA.02\State=1-A\HF=-326.9631487\RMSD=7.722e-  
09\Dipole=0.3946621,0.034519,0.3006968\Quadrupole=1.1567054,-  
2.4291498,1.2724444,3.9209199,-0.3281783,2.8671346\PG=C01 [X(C7H9N1)]\@

HF=-326.933578

Sum of electronic and zero-point Energies= -326.789043  
 Sum of electronic and thermal Energies= -326.781337  
 Sum of electronic and thermal Enthalpies= -326.780393  
 Sum of electronic and thermal Free Energies= -326.821367  
 NImag=0

C6H6Cl1N1

-----  
 0,1  
 N,0.0186384264,-0.0497009318,0.0143994879  
 H,-0.0382100489,0.090588856,1.0148832006  
 H,0.9424499598,0.1292241843,-0.3590506066  
 C,-0.6353340244,-1.1740917601,-0.4765384775  
 C,-0.2963324641,-1.7543112274,-1.7139210977  
 C,-1.7160764532,-1.7448777636,0.2241520233  
 C,-0.9936073599,-2.8436642977,-2.2322039827  
 C,-2.4167617194,-2.8335307026,-0.2874191873  
 C,-2.0618545515,-3.3910994191,-1.5202776427  
 Cl,1.057324928,-1.0882233337,-2.6321715477  
 H,-2.0040212495,-1.3111900934,1.1795774553  
 H,-0.6924059209,-3.2566359436,-3.189956583  
 H,-3.2453346423,-3.2478078074,0.2809241454  
 H,-2.6052716419,-4.2399067029,-1.9244851485

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RB3LYP\6-31+G(d)\C6H6Cl1N1\ROSMUS\03-Jan-2012\0\#p b3lyp 6-31+G\* opt=(noeigen) freq\3-Chloroaniline\0,1\N,0.0186384264,-0.0497009318,0.0143994879\H,-0.0382100489,0.090588856,1.0148832006\H,0.9424499598,0.1292241843,-0.3590506066\C,-0.6353340244,-1.1740917601,-0.4765384775\C,-0.2963324641,-1.7543112274,-1.7139210977\C,-1.7160764532,-1.7448777636,0.2241520233\C,-0.9936073599,-2.8436642977,-2.2322039827\C,-2.4167617194,-2.8335307026,-0.2874191873\C,-2.0618545515,-3.3910994191,-1.5202776427\Cl,1.057324928,-1.0882233337,-2.6321715477\H,-2.0040212495,-1.3111900934,1.1795774553\H,-0.6924059209,-3.2566359436,-3.189956583\H,-3.2453346423,-3.2478078074,0.2809241454\H,-2.6052716419,-4.2399067029,-1.9244851485\Version=IA64L-G09RevA.02\State=1-A\HF=-747.2131668\RMSD=5.944e-09\RMSF=2.246e-05\Dipole=-0.0570359,-0.0778568,0.7659279\Quadrupole=-0.7918708,-1.4758906,2.2677614,3.4183761,0.3514515,3.8088849\PG=C01 [X(C6H6Cl1N1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RB3LYP\Aug-CC-pVDZ\C6H6Cl1N1\ROSMUS\03-Jan-2012\0\#p b3lyp aug-cc-pvdz geom=allcheck guess=read scf=verytight pop=savenbos\3-Chloroaniline\0,1\N,0,0.0186384264,-

0.0497009318,0.0143994879\H,0,-  
0.0382100489,0.090588856,1.0148832006\H,0,0.9424499598,0.1292241843,-  
0.3590506066\C,0,-0.6353340244,-1.1740917601,-0.4765384775\C,0,-0.2963324641,-  
1.7543112274,-1.7139210977\C,0,-1.7160764532,-1.7448777636,0.2241520233\C,0,-  
0.9936073599,-2.8436642977,-2.2322039827\C,0,-2.4167617194,-2.8335307026,-  
0.2874191873\C,0,-2.0618545515,-3.3910994191,-1.5202776427\C1,0,1.057324928,-  
1.0882233337,-2.6321715477\H,0,-2.0040212495,-1.3111900934,1.1795774553\H,0,-  
0.6924059209,-3.2566359436,-3.189956583\H,0,-3.2453346423,-  
3.2478078074,0.2809241454\H,0,-2.6052716419,-4.2399067029,-  
1.9244851485\\Version=IA64L-G09RevA.02\State=1-A\HF=-  
747.2648484\RMSD=5.150e-09\Dipole=-0.0658907,-  
0.0473427,0.7246915\Quadrupole=-0.8517764,-  
1.3108557,2.1626321,3.10437,0.3203157,3.6123912\PG=C01 [X(C6H6C11N1)]\@

HF=-747.1807089

Sum of electronic and zero-point Energies= -747.105382  
Sum of electronic and thermal Energies= -747.098480  
Sum of electronic and thermal Enthalpies= -747.097536  
Sum of electronic and thermal Free Energies= -747.136654  
NImag=0

C6H6F1N1

-----

0,1  
N  
H,1,r2  
H,1,r3,2,a3  
C,1,r8,2,a8,3,d8,0  
C,4,r9,1,a9,3,d9,0  
C,4,r10,1,a10,5,d10,0  
C,5,r11,4,a11,1,d11,0  
C,6,r12,4,a12,1,d12,0  
C,7,r13,5,a13,1,d13,0  
H,5,r14,4,a14,9,d14,0  
H,6,r15,4,a15,9,d15,0  
H,7,r16,5,a16,9,d16,0  
H,8,r17,6,a17,9,d17,0  
F,9,r18,7,a18,8,d18,0

r2=1.00806639  
r3=1.00806514  
r8=1.39799987  
r9=1.39445066  
r10=1.39446142

r11=1.38603432  
r12=1.38602047  
r13=1.37956913  
r14=1.08298349  
r15=1.08298523  
r16=1.08111434  
r17=1.08111277  
r18=1.34382452  
a3=111.25353563  
a8=114.57171216  
a9=120.67337775  
a10=120.66913518  
a11=120.90670754  
a12=120.90809235  
a13=119.03061124  
a14=119.44571802  
a15=119.44313792  
a16=121.33717037  
a17=121.33870616  
a18=119.23495935  
d8=131.94649511  
d9=-26.31749868  
d10=-176.98377328  
d11=-177.30595977  
d12=177.28354078  
d13=-2.56092617  
d14=179.69584534  
d15=-179.68957743  
d16=-180.02660587  
d17=179.99788954  
d18=-179.91448582

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C6H6F1N1\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\N\H,1,r2\H,1,r3,2,a3\C,1,r8,2,a8,3,d8,0\C,4,r9,1,a9,3,d9,0\C,4,r10,1,a10,5,d10,0\C,5,r11,4,a11,1,d11,0\C,6,r12,4,a12,1,d12,0\C,7,r13,5,a13,1,d13,0\H,5,r14,4,a14,9,d14,0\H,6,r15,4,a15,9,d15,0\H,7,r16,5,a16,9,d16,0\H,8,r17,6,a17,9,d17,0\F,9,r18,7,a18,8,d18,0\r2=1.00806639\r3=1.00806514\r8=1.39799987\r9=1.39445066\r10=1.39446142\r11=1.38603432\r12=1.38602047\r13=1.37956913\r14=1.08298349\r15=1.08298523\r16=1.08111434\r17=1.08111277\r18=1.34382452\a3=111.25353563\a8=114.57171216\a9=120.67337775\a10=120.66913518\a11=120.90670754\a12=120.90809235\a13=119.03061124\a14=119.44571802\a15=119.44313792\a16=121.33717037\a17=121.33870616\a18=119.23495935\d8=131.94649511\d9=-26.31749868\d10=-176.98377328\d11=-177.30595977\d12=177.28354078\d13=-2.56092617\d14=179.69584534\d15=-179.68957743\d16=-180.02660587\d17=179.99788954\d18=-

179.91448582\\Version=IA64L-G09RevA.02\\State=1-A\\HF=-  
386.8196738\\RMSD=9.645e-09\\RMSF=3.544e-  
05\\Dipole=0.8651827,0.3749924,0.5917981\\Quadrupole=1.9923704,-  
5.1668235,3.174453,1.2270916,-1.5243196,0.84221\\PG=C01 [X(C6H6F1N1)]\\@  
--- NBO Single Point ---  
1\\1\\GINC-PAULING\\SP\\RHF\\CC-pVQZ\\C6H6F1N1\\ROSMUS\\20-Jul-2012\\0\\#p  
hf/cc-pvqz scf=verytight pop=(nboread) guess=read  
geom=allcheck\\title\\0,1\\N\\H,1,1.0080663949\\H,1,1.0080651378,2,111.25353563\\C,1,1.  
397999868,2,114.57171216,3,131.94649511,0\\C,4,1.3944506629,1,120.67337775,3,-  
26.31749868,0\\C,4,1.3944614241,1,120.66913518,5,-  
176.98377328,0\\C,5,1.3860343241,4,120.90670754,1,-  
177.30595977,0\\C,6,1.3860204709,4,120.90809235,1,177.28354078,0\\C,7,1.379569130  
1,5,119.03061124,1,-  
2.56092617,0\\H,5,1.0829834913,4,119.44571802,9,179.69584534,0\\H,6,1.0829852329,4  
,119.44313792,9,-179.68957743,0\\H,7,1.0811143407,5,121.33717037,9,-  
180.02660587,0\\H,8,1.0811127738,6,121.33870616,9,179.99788954,0\\F,9,1.343824516  
7,7,119.23495935,8,-179.91448582,0\\Version=IA64L-G09RevA.02\\State=1-A\\HF=-  
384.7471879\\RMSD=6.836e-  
09\\Dipole=0.8895275,0.3744736,0.608456\\Quadrupole=2.0343764,-  
5.415843,3.3814666,1.012258,-1.7366805,0.6954061\\PG=C01 [X(C6H6F1N1)]\\@

HF=-386.8196738

Sum of electronic and zero-point Energies= -386.709956  
Sum of electronic and thermal Energies= -386.703428  
Sum of electronic and thermal Enthalpies= -386.702484  
Sum of electronic and thermal Free Energies= -386.740379  
NImag=0

C6H7N1

-----

0,1  
N  
H,1,r2  
H,1,r3,2,a3  
C,1,r8,2,a8,3,d8,0  
C,4,r9,1,a9,3,d9,0  
C,4,r10,1,a10,5,d10,0  
C,5,r11,4,a11,1,d11,0  
C,6,r12,4,a12,1,d12,0  
C,7,r13,5,a13,1,d13,0  
H,5,r14,4,a14,9,d14,0  
H,6,r15,4,a15,9,d15,0  
H,7,r16,5,a16,9,d16,0  
H,8,r17,6,a17,9,d17,0

H,9,r18,7,a18,8,d18,0

r2=1.00764152  
r3=1.00764193  
r8=1.39387007  
r9=1.39541831  
r10=1.39543597  
r11=1.38521624  
r12=1.38519797  
r13=1.38831496  
r14=1.08339288  
r15=1.08339593  
r16=1.08226435  
r17=1.08226054  
r18=1.08068092  
a3=111.90607593  
a8=115.07781194  
a9=120.5851106  
a10=120.58376266  
a11=120.39176434  
a12=120.39354728  
a13=120.77522141  
a14=119.34544419  
a15=119.3435671  
a16=119.24637961  
a17=119.24832664  
a18=120.55675163  
d8=133.83260196  
d9=-25.24280989  
d10=-177.16392583  
d11=-177.38072517  
d12=177.37354069  
d13=-2.50171684  
d14=179.70129549  
d15=-179.70053829  
d16=-179.99569177  
d17=179.98863918  
d18=-179.97412707

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C6H7N1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\0,1\N\H,1,r2\H,1,r3,2,a3\C,1,r8,2,a8,3,d8,0\C,4,r9,1,a9,3,d9,0\C,4,r10,1,a10,5,d10,0\C,5,r11,4,a11,1,d11,0\C,6,r12,4,a12,1,d12,0\C,7,r13,5,a13,1,d13,0\H,5,r14,4,a14,9,d14,0\H,6,r15,4,a15,9,d15,0\H,7,r16,5,a16,9,d16,0\H,8,r17,6,a17,9,d17,0\H,9,r18,7,a18,8,d18,0\r2=1.00764152\r3=1.00764193\r8=1.39387007\r9=1.39541831\r10=1.39543597\r11=



1.38521624\r12=1.38519797\r13=1.38831496\r14=1.08339288\r15=1.08339593\r16=1.08226435\r17=1.08226054\r18=1.08068092\aa3=111.90607593\aa8=115.07781194\aa9=120.5851106\aa10=120.58376266\aa11=120.39176434\aa12=120.39354728\aa13=120.77522141\aa14=119.34544419\aa15=119.3435671\aa16=119.24637961\aa17=119.24832664\aa18=120.55675163\dd8=133.83260196\dd9=-25.24280989\dd10=-177.16392583\dd11=-177.38072517\dd12=177.37354069\dd13=-2.50171684\dd14=179.70129549\dd15=-179.70053829\dd16=-179.99569177\dd17=179.98863918\dd18=-179.97412707\Version=IA64L-G09RevA.02\State=1-A\HF=-287.5733364\RMSD=9.579e-09\RMSF=1.714e-05\Dipole=0.4913428,-0.0058294,0.3320139\Quadrupole=2.1636986,-4.387173,2.2234744,3.0664665,-0.0744918,2.0716984\PG=C01 [X(C6H7N1)]\@\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C6H7N1\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) guess=read  
 geom=allcheck\0,1\N\H,1,1.0076415233\H,1,1.0076419308,2,111.90607593\C,1,1.3938700739,2,115.07781194,3,133.83260196,0\C,4,1.3954183146,1,120.5851106,3,-25.24280989,0\C,4,1.3954359714,1,120.58376266,5,-177.16392583,0\C,5,1.3852162365,4,120.39176434,1,-177.38072517,0\C,6,1.3851979653,4,120.39354728,1,177.37354069,0\C,7,1.3883149555,5,120.77522141,1,-2.50171684,0\H,5,1.0833928751,4,119.34544419,9,179.70129549,0\H,6,1.0833959305,4,119.3435671,9,-179.70053829,0\H,7,1.0822643535,5,119.24637961,9,-179.99569177,0\H,8,1.0822605375,6,119.24832664,9,179.98863918,0\H,9,1.0806809153,7,120.55675163,8,-179.97412707,0\Version=IA64L-G09RevA.02\State=1-A\HF=-285.851659\RMSD=5.919e-09\Dipole=0.4743995,-0.0464697,0.3205733\Quadrupole=2.2280047,-4.578897,2.3508923,3.0671718,-0.1530065,2.0721673\PG=C01 [X(C6H7N1)]\@\@

HF=-287.5733364

Sum of electronic and zero-point Energies= -287.455684  
 Sum of electronic and thermal Energies= -287.449942  
 Sum of electronic and thermal Enthalpies= -287.448998  
 Sum of electronic and thermal Free Energies= -287.484777  
 NImag=0

C6H7N1O1

-----  
 0,1  
 N  
 H,1,r2  
 H,1,r3,2,a3  
 C,1,r8,2,a8,3,d8,0  
 C,4,r9,1,a9,3,d9,0  
 C,4,r10,1,a10,5,d10,0

C,5,r11,4,a11,1,d11,0  
C,6,r12,4,a12,1,d12,0  
C,7,r13,5,a13,1,d13,0  
H,5,r14,4,a14,9,d14,0  
H,6,r15,4,a15,9,d15,0  
H,7,r16,5,a16,9,d16,0  
H,8,r17,6,a17,9,d17,0  
O,9,r18,7,a18,8,d18,0  
H,14,r19,9,a19,7,d19,0

r2=1.00864458  
r3=1.00867877  
r8=1.4029986  
r9=1.39443165  
r10=1.3910483  
r11=1.3837519  
r12=1.38779723  
r13=1.38784827  
r14=1.0833986  
r15=1.08325413  
r16=1.08145263  
r17=1.08407176  
r18=1.36642206  
r19=0.959134  
a3=110.59275033  
a8=114.05155922  
a9=120.74745219  
a10=120.99838644  
a11=121.12167356  
a12=120.89237687  
a13=120.15475003  
a14=119.35021644  
a15=119.55133478  
a16=120.91978862  
a17=119.73409085  
a18=117.7258743  
a19=109.74035686  
d8=129.90767278  
d9=-27.51076886  
d10=-176.82711089  
d11=-177.18323827  
d12=177.15151932  
d13=-2.69051279  
d14=179.66559634  
d15=-179.66031906  
d16=-180.04718456

d17=180.00164994  
d18=-179.90427002  
d19=-179.53711917

--- Geometry Optimization ---

```
1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C6H7N1O1\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\N\H,1,r2\H,1,r3,2,a3\C,1,r8,2,a8,3,d8,0\C,4,r9,1,a9,3,d9,0\C,4,r10,1,a10,5,
d10,0\C,5,r11,4,a11,1,d11,0\C,6,r12,4,a12,1,d12,0\C,7,r13,5,a13,1,d13,0\H,5,r14,4,a14,9,
d14,0\H,6,r15,4,a15,9,d15,0\H,7,r16,5,a16,9,d16,0\H,8,r17,6,a17,9,d17,0\O,9,r18,7,a18,8,
,d18,0\H,14,r19,9,a19,7,d19,0\r2=1.00864458\r3=1.00867877\r8=1.4029986\r9=1.3944
3165\r10=1.3910483\r11=1.3837519\r12=1.38779723\r13=1.38784827\r14=1.0833986\r
15=1.08325413\r16=1.08145263\r17=1.08407176\r18=1.36642206\r19=0.959134\
a3=110.59275033\
a8=114.05155922\
a9=120.74745219\
a10=120.99838644\
a11=121.12167356\
a12=120.89237687\
a13=120.15475003\
a14=119.35021644\
a15=119.55133478\
a16=120.91978862\
a17=119.73409085\
a18=117.7258743\
a19=109.74035686\
d8=129.90767278\
d9=-27.51076886\
d10=-176.82711089\
d11=-177.18323827\
d12=177.15151932\
d13=-2.69051279\
d14=179.66559634\
d15=-179.66031906\
d16=-180.04718456\
d17=180.00164994\
d18=-179.90427002\
d19=-179.53711917\
\Version=IA64L-G09RevA.02\State=1-A\HF=-362.8003006\
RMSD=3.625e-09\RMSF=6.486e-05\Dipole=0.1916329,-0.0159857,0.7465269\
Quadrupole=4.7386889,-4.9416953,0.2030064,4.381102,-1.6756807,0.0639335\
PG=C01 [X(C6H7N1O1)]\@\
```

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C6H7N1O1\ROSMUS\20-Jul-2012\0\#\#p
hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck
guess=read\title\0,1\N\H,1,1.0086445832\H,1,1.0086787673,2,110.59275033\C,1,1.402
9985969,2,114.05155922,3,129.90767278,0\C,4,1.3944316516,1,120.74745219,3,-
27.51076886,0\C,4,1.3910482952,1,120.99838644,5,-
176.82711089,0\C,5,1.3837519046,4,121.12167356,1,-
177.18323827,0\C,6,1.3877972302,4,120.89237687,1,177.15151932,0\C,7,1.387848271
5,5,120.15475003,1,-
2.69051279,0\H,5,1.0833986001,4,119.35021644,9,179.66559634,0\H,6,1.083254131,4,
119.55133478,9,-179.66031906,0\H,7,1.0814526272,5,120.91978862,9,-
180.04718456,0\H,8,1.0840717602,6,119.73409085,9,180.00164994,0\O,9,1.366422058
6,7,117.7258743,8,-179.90427002,0\H,14,0.959133996,9,109.74035686,7,-
179.53711917,0\Version=IA64L-G09RevA.02\State=1-A\HF=-360.743206\
RMSD=7.732e-09\Dipole=0.1950577,-0.0290761,0.7667882\
Quadrupole=4.885265,-5.1839209,0.2986558,4.2830906,-1.8602936,-0.1013785\
PG=C01 [X(C6H7N1O1)]\@\
```

HF=-362.8003006

Sum of electronic and zero-point Energies=	-362.678356
Sum of electronic and thermal Energies=	-362.671358
Sum of electronic and thermal Enthalpies=	-362.670413

Sum of electronic and thermal Free Energies= -362.709047  
NImag=0

## Other Donors

As1H3O1

-----  
0,1  
O  
As,1,r2  
X,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0

r2=1.80081016  
r4=0.95832033  
r5=1.52328401  
a4=109.75328284  
a5=95.8280133  
d4=120.78056979  
d5=223.27553049  
r6=1.52476573  
a6=96.3085223  
d6=130.78977849  
r3=1.0154182  
a3=104.68557609

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\As1H3O1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\As,1,r2\X,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\r2=1.80081016\r4=0.95832033\r5=1.52328401\a4=109.75328284\a5=95.8280133\d4=120.78056979\d5=223.27553049\r6=1.52476573\a6=96.3085223\d6=130.78977849\r3=1.0154182\a3=104.68557609\Version=IA64L-G09RevA.02\State=1-A\HF=-2312.8750151\RMSD=3.549e-09\RMSF=1.355e-04\Dipole=-0.172814,-0.3035761,0.258262\Quadrupole=0.0858475,0.4506588,-0.5365063,0.1959811,1.5381959,2.5219533\PG=C01 [X(As1H3O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\As1H3O1\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nbread) geom=allcheck  
guess=read\title\0,1\O\As,1,1.8008101645\X,1,1.0154182,2,104.68557609\H,1,0.9583203314,2,109.75328284,3,120.78056979,0\H,2,1.5232840144,1,95.8280133,4,223.27553049,0\H,2,1.52476573,1,96.3085223,4,130.78977849,0\Version=IA64L-

G09RevA.02\State=1-A\HF=-2310.8849328\RMSD=7.197e-09\Dipole=-0.1869514,-  
0.3276049,0.2901919\Quadrupole=0.161133,0.4639103,-  
0.6250433,0.1259548,1.5897675,2.6067086\PG=C01 [X(As1H3O1)]\@

HF=-2312.8750151

Sum of electronic and zero-point Energies= -2312.845147  
Sum of electronic and thermal Energies= -2312.841504  
Sum of electronic and thermal Enthalpies= -2312.840560  
Sum of electronic and thermal Free Energies= -2312.870546  
NImag=0

Br1H1O1

-----

0,1  
O  
Br,1,r2  
H,1,r3,2,a3

r2=1.81530123  
r3=0.96343211  
a3=104.54780877

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Br1H1O1\ROSMUS\23-Jul-  
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Br,1,r2\H,1,r3,2,a3\r2=1.81530123\r3=0.96343211\a3=104.54780877\  
Version=IA64L-G09RevA.02\State=1-A\HF=-2649.9414499\RMSD=4.290e-  
09\RMSF=1.098e-04\Dipole=0.5741924,0.,-0.0077287\Quadrupole=0.3595004,-  
1.3689741,1.0094737,0.,-2.3500989,0.\PG=CS [SG(Br1H1O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br1H1O1\ROSMUS\23-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\Br,1,1.8153012273\H,1,0.9634321147,2,104.54780877\Version  
=IA64L-G09RevA.02\State=1-A\HF=-2647.8873423\RMSD=4.862e-  
09\Dipole=0.6030068,0.,0.0267071\Quadrupole=0.3615552,-1.3165767,0.9550215,0.,-  
2.3964008,0.\PG=CS [SG(Br1H1O1)]\@

HF=-2649.9414499

Sum of electronic and zero-point Energies= -2649.928294  
Sum of electronic and thermal Energies= -2649.925330  
Sum of electronic and thermal Enthalpies= -2649.924386  
Sum of electronic and thermal Free Energies= -2649.952419  
NImag=0

C1H4O1

-----  
0,1  
O  
Cl,1,r2  
H,1,r3,2,a3

r2=1.67205684  
r3=0.96367204  
a3=104.56506389

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C1H1O1\ROSMUS\23-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Cl,1,r2\H,1,r3,2,a3\r2=1.67205684\r3=0.96367204\a3=104.56506389\  
Version=IA64L-G09RevA.02\State=1-A\HF=-535.9580391\RMSD=2.583e-  
09\RMSF=6.487e-05\Dipole=0.6052863,0.,-0.1340683\Quadrupole=0.4767828,-  
1.2266252,0.7498424,0.,-1.942379,0.\PG=CS [SG(C1H1O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C1H4O1\ROSMUS\25-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\C,1,1.4119098429\H,1,0.9576247643,2,109.17502126\H,2,1.087  
685577,1,106.94346869,3,180.,0\H,2,1.0931433299,1,112.01760954,3,61.42839604,0\H,  
2,1.0931433299,1,112.01760954,3,-61.42839604,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-115.0991227\RMSD=2.754e-  
09\Dipole=0.5649801,0.,0.3984874\Quadrupole=0.90174,-0.5849613,-0.3167787,0.,-  
1.6114949,0.\PG=CS [SG(C1H2O1),X(H2)]\@

HF=-115.7125047

Sum of electronic and zero-point Energies= -115.660798  
Sum of electronic and thermal Energies= -115.657404  
Sum of electronic and thermal Enthalpies= -115.656460  
Sum of electronic and thermal Free Energies= -115.683617  
NImag=0

C1H1O1

-----  
0,1  
O  
Cl,1,r2  
H,1,r3,2,a3

r2=1.67205684  
r3=0.96367204  
a3=104.56506389

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C11H1O1\ROSMUS\23-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\C1,1,r2\H,1,r3,2,a3\r2=1.67205684\r3=0.96367204\a3=104.56506389\Version=IA64L-G09RevA.02\State=1-A\HF=-535.9580391\RMSD=2.583e-09\RMSF=6.487e-05\Dipole=0.6052863,0.,-0.1340683\Quadrupole=0.4767828,-1.2266252,0.7498424,0.,-1.942379,0.\PG=CS [SG(C11H1O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C11H1O1\ROSMUS\23-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\C1,1,1.6720568385\H,1,0.96367204,2,104.56506389\Version=IA64L-G09RevA.02\State=1-A\HF=-534.9314633\RMSD=9.134e-09\Dipole=0.6345532,0.,-0.122743\Quadrupole=0.4617315,-1.1884581,0.7267266,0.,-1.9784767,0.\PG=CS [SG(C11H1O1)]\@

HF=-535.9580391

Sum of electronic and zero-point Energies=	-535.944434
Sum of electronic and thermal Energies=	-535.941517
Sum of electronic and thermal Enthalpies=	-535.940573
Sum of electronic and thermal Free Energies=	-535.967334

NImag=0

F1H1O1

-----  
0,1  
O  
F,1,r2  
H,1,r3,2,a3

r2=1.394821  
r3=0.96711229  
a3=99.64501774

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\F1H1O1\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\F,1,r2\H,1,r3,2,a3\r2=1.394821\r3=0.96711229\a3=99.64501774\Version=IA64L-G09RevA.02\State=1-A\HF=-175.5352466\RMSD=9.461e-09\RMSF=8.467e-05\Dipole=0.6811448,0.,-0.349917\Quadrupole=0.8475316,-0.8473921,-0.0001394,0.,-1.2572037,0.\PG=CS [SG(F1H1O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F1H1O1\ROSMUS\20-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\F,1,1.3948210045\H,1,0.967112294,2,99.64501774\Version=IA  
64L-G09RevA.02\State=1-A\HF=-174.8212515\RMSD=7.405e-  
09\Dipole=0.7153993,0.,-0.4243462\Quadrupole=0.8910603,-0.790975,-0.1000853,0.,-  
1.2893235,0.\PG=CS [SG(F1H1O1)]\@

HF=-175.5352466

Sum of electronic and zero-point Energies=	-175.520733
Sum of electronic and thermal Energies=	-175.517868
Sum of electronic and thermal Enthalpies=	-175.516924
Sum of electronic and thermal Free Energies=	-175.542557
NImag=0	

Ge1H4O1

-----

0,1  
O  
Ge,1,r2  
X,1,1.,2,110.65  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.7865212  
r4=0.95722077  
a4=115.14860647  
d4=17.82812184  
r5=1.54398731  
r6=1.5439294  
r7=1.53519637  
a5=109.7507251  
a6=109.76476517  
a7=104.49158865  
d5=59.79524458  
d6=-60.84307227  
d7=179.49403735

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Ge1H4O1\ROSMUS\23-Jul-  
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Ge,1,r2\X,1,1.,2,110.65\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a



6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.7865212\r4=0.95722077\a4=115.14860647\d4=17.828  
12184\r5=1.54398731\r6=1.5439294\r7=1.53519637\a5=109.75072519\a6=109.7647651  
7\a7=104.49158865\d5=59.79524458\d6=-  
60.84307227\d7=179.49403735\\Version=IA64L-G09RevA.02\State=1-A\HF=-  
2154.6082433\RMSD=8.766e-09\RMSF=2.402e-05\Dipole=0.4710188,-  
0.1512596,0.3235189\Quadrupole=0.8132694,-0.4411107,-0.3721587,-0.4514832,-  
2.3217798,0.7488527\PG=C01 [X(Ge1H4O1)]\@  
--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge1H4O1\ROSMUS\23-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\Ge,1,1.7865211988\X,1,1.,2,110.65\H,1,0.9572207743,2,115.14  
860647,3,17.82812184,0\H,2,1.5439873065,1,109.75072519,4,59.79524458,0\H,2,1.543  
9294026,1,109.76476517,4,-  
60.84307227,0\H,2,1.5351963684,1,104.49158865,4,179.49403735,0\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-2152.6516502\RMSD=3.876e-09\Dipole=0.4975288,-  
0.1598055,0.3468615\Quadrupole=0.8277592,-0.3877205,-0.4400387,-0.4374309,-  
2.3730235,0.7652955\PG=C01 [X(Ge1H4O1)]\@

HF=-2154.6082433

Sum of electronic and zero-point Energies= -2154.571348  
Sum of electronic and thermal Energies= -2154.567288  
Sum of electronic and thermal Enthalpies= -2154.566344  
Sum of electronic and thermal Free Energies= -2154.597224  
NImag=0

H3N1O1

-----  
0,1  
O  
N,1,r2  
X,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0

r2=1.42005756  
r4=0.95863577  
r5=1.0154071  
a4=103.47676675  
a5=104.68727348  
d4=140.32219334  
d5=235.72214186  
r6=1.01541229  
a6=104.6884171

d6=124.27295832  
r3=1.0154182  
a3=104.68557609

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\H3N1O1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\N,1,r2\X,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\r2=1.42005756\r4=0.95863577\r5=1.0154071\a4=103.47676675\a5=104.68727348\d4=140.32219334\d5=235.72214186\r6=1.01541229\a6=104.6884171\d6=124.27295832\r3=1.0154182\a3=104.68557609\Version=IA64L-G09RevA.02\State=1-A\HF=-131.7129021\RMSD=6.895e-09\RMSF=1.456e-05\Dipole=0.0240563,0.0199206,0.2218891\Quadrupole=0.3168826,0.2704921,-0.5873747,0.1237969,2.1945009,1.8203654\PG=C01 [X(H3N1O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3N1O1\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\N,1,1.4200575559\X,1,1.0154182,2,104.68557609\H,1,0.9586357728,2,103.47676675,3,140.32219334,0\H,2,1.0154070967,1,104.68727348,4,235.72214186,0\H,2,1.0154122868,1,104.6884171,4,124.27295832,0\Version=IA64L-G09RevA.02\State=1-A\HF=-131.0532817\RMSD=5.448e-09\Dipole=0.0227231,0.0188131,0.2566899\Quadrupole=0.3603361,0.3112127,-0.6715488,0.1310551,2.2295076,1.8494048\PG=C01 [X(H3N1O1)]\@

HF=-131.7129021

Sum of electronic and zero-point Energies=	-131.671804
Sum of electronic and thermal Energies=	-131.668646
Sum of electronic and thermal Enthalpies=	-131.667702
Sum of electronic and thermal Free Energies=	-131.694208
NImag=0	

H2O2

-----  
0,1  
O  
O,1,r2  
O,1,r3,2,a3  
X,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.39608124  
r3=1.39591533  
r5=0.96594198

r6=0.9659482  
a3=107.35364818  
a5=103.1368394  
a6=103.14762872  
d5=200.64716833  
d6=266.05759736

r4=1.  
a4=101.913  
d4=106.634

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H2O3\ROSMUS\14-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\O,1,r2\O,1,r3,2,a3\X,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\r2=1.39608124\r3=1.39591533\r5=0.96594198\r6=0.9659482\a3=107.35364818\a5=103.1368394\a6=103.14762872\d5=200.64716833\d6=266.05759736\r4=1.\a4=101.913\d4=106.634\Version=IA64L-G09RevA.02\State=1-A\HF=-226.6847501\RMSD=4.062e-09\RMSF=1.869e-04\Dipole=0.1548598,1.2484696,0.1141826\Quadrupole=-0.9099116,1.2848521,-0.3749405,0.7447006,-0.861634,0.5485236\PG=C01 [X(H2O3)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H2O2\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\O,1,1.4179551186\X,1,1.0154182,2,104.68557609\H,1,0.9630183354,2,101.71827421,3,73.34835468,0\H,2,0.9630161031,1,101.71893572,4,249.42820532,0\Version=IA64L-G09RevA.02\State=1-A\HF=-150.8504913\RMSD=6.428e-09\Dipole=-0.4755087,-0.5949319,0.0000048\Quadrupole=0.3555422,0.0415162,-0.3970584,-0.6949715,-1.7566124,1.4039966\PG=C01 [X(H2O2)]\@

HF=-151.5461933

Sum of electronic and zero-point Energies= -151.518807  
Sum of electronic and thermal Energies= -151.515619  
Sum of electronic and thermal Enthalpies= -151.514675  
Sum of electronic and thermal Free Energies= -151.541037  
NImag=0

H3O1P1

-----  
O,1  
P  
O,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

H,2,r5,1,a5,4,d5,0

r2=1.65587874  
r3=1.41296521  
r4=1.41376698  
r5=0.95807093  
a3=98.23733652  
a4=98.22410906  
a5=110.4819954  
d4=93.79686123  
d5=227.78594524

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O1P1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\r2=1.65587874  
\r3=1.41296521\r4=1.41376698\r5=0.95807093\ a3=98.23733652\ a4=98.22410906\ a5=110.4819954\ d4=93.79686123\ d5=227.78594524\ \Version=IA64L-G09RevA.02\State=1-A\HF=-418.3675144\RMSD=3.274e-09\RMSF=1.554e-04\Dipole=-0.1986257,0.2018052,-0.0025234\Quadrupole=0.1559365,0.1344484,-0.2903849,-0.2412193,-1.9872189,2.0736998\PG=C01 [X(H3O1P1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O1P1\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O,1,1.6558787405\H,1,1.4129652058,2,98.23733652\H,1,1.4137669827,2,98.22410906,3,93.79686123,0\H,2,0.9580709273,1,110.4819954,4,227.78594524,0\ \Version=IA64L-G09RevA.02\State=1-A\HF=-417.4072035\RMSD=4.438e-09\Dipole=-0.1988677,0.2015889,-0.0343446\Quadrupole=0.1905927,0.1582869,-0.3488796,-0.1583171,-2.0716647,2.1627113\PG=C01 [X(H3O1P1)]\@\

HF=-418.3675144

Sum of electronic and zero-point Energies= -418.335417  
Sum of electronic and thermal Energies= -418.331974  
Sum of electronic and thermal Enthalpies= -418.331029  
Sum of electronic and thermal Free Energies= -418.359377  
NImag=0

H2O1Se1

-----  
0,1  
O  
Se,1,r2  
H,1,r4,2,a4  
H,2,r5,1,a5,3,d5,0

r2=1.80020785  
r4=0.96029661  
r5=1.47262396  
a4=107.799023  
a5=96.44073216  
d5=269.83644174

--- Geometry Optimization ---

```
1\1\GINC-PAULING\Freq\RM062X\6-311++G(3df,2p)\H2O1Se1\ROSMUS\25-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(calcall,z-matrix,noeigen) scf=(fermi,xqc) optcyc=100  
freq\title\0,1\O\Se,1,r2\H,1,r4,2,a4\H,2,r5,1,a5,3,d5,0\r2=1.80020785\r4=0.96029661\r5=1.47262396\ a4=107.799023\ a5=96.44073216\ d5=269.83644174\Version=IA64L-G09RevA.02\State=1-A\HF=-2477.9493913\RMSD=8.824e-09\RMSF=1.390e-04\ZeroPoint=0.0216704\Thermal=0.0249806\Dipole=0.5377231,-0.2338216,0.1496104\DipoleDeriv=-0.288209,-0.0131735,0.1742122,-0.0037862,-0.447932,-0.0743476,0.0772266,0.0990197,-1.0011296,-0.0208909,-0.0017891,-0.0535996,-0.0036022,0.2726867,0.0314801,-0.0514462,-0.0672692,0.777465,0.2271135,0.012091,-0.1221616,0.0080346,0.3088826,-0.0048571,-0.0330829,-0.0009665,0.247705,0.0819864,0.0028716,0.001549,-0.0006462,-0.1336373,0.0477246,0.0073026,-0.030784,-0.0240404\Polar=31.7744428,0.0874729,31.6119875,-0.7464534,-1.3872893,37.1160066\PG=C01  
[X(H2O1Se1)]\NImag=0\0.52626374,0.00149088,0.02333745,-0.14940525,-0.00974542,0.30826525,-0.02015574,-0.00251926,-0.01027386,0.01468068,-0.00030857,-0.02384869,0.00515148,0.00097626,0.25550698,0.02441718,-0.01106745,-0.22490276,-0.01476826,-0.00284311,0.26582096,-0.50542503,-0.00166873,0.16003987,0.00596890,0.00037884,-0.01099383,0.49946886,-0.00075595,-0.00471942,0.00019649,0.00282981,-0.00017002,-0.00135620,0.00093825,0.00535613,0.12376069,0.00051574,-0.07199919,0.02361798,0.00009667,-0.02338281,-0.14808513,-0.00059958,0.09565177,-0.00068298,0.00269712,-0.00036076,-0.00049384,-0.00104653,0.00134491,-0.00001273,-0.00301211,0.00070646,0.00118955,-0.00042636,0.00523066,0.00439745,-0.00128681,-0.23148827,0.01526677,0.00035164,-0.00046669,-0.00001283,0.00136153,0.22672430,0.00122737,0.02029714,-0.01136330,0.00142414,-0.00240504,-0.01753539,-0.00096092,0.00175929,-0.00026977,-0.00169060,-0.01965139,0.02916845\0.00024585,-0.00005958,0.00000317,-0.00036825,0.00011894,-0.00000410,0.00000109,-0.00005902,-0.00000130,0.00012131,-0.00000033,0.00000222\ \@
```

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H2O1Se1\ROSMUS\25-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\O\Se,1,1.80020785\H,1,0.96029661\O3,2,107.799023\H,2,1.472623962,1,96.44073216,3,269.83644174,0\Version=IA64L-G09RevA.02\State=1-A\HF=-2475.9250947\RMSD=6.009e-09\Dipole=0.570317,-0.2535244,0.1965447\Quadrupole=-
```

0.7451145,0.6020027,0.1431118,0.0691371,-2.401909,-0.5657447\PG=C01  
[X(H2O1Se1)]\@

HF=-2477.9493913

Sum of electronic and zero-point Energies= -2477.927721  
Sum of electronic and thermal Energies= -2477.924411  
Sum of electronic and thermal Enthalpies= -2477.923467  
Sum of electronic and thermal Free Energies= -2477.952634  
NImag=0

H4O1Si1

-----  
0,1  
O  
Si,1,rS  
H,1,rO,2,aO  
H,2,ra,1,aa,3,da,0  
H,2,rH,1,aH,3,dH,0  
H,2,rH,1,aH,3,-dH,0

rS=1.64753915  
rO=0.95620541  
ra=1.4708587  
rH=1.47774506  
aO=119.08623721  
aa=105.99841362  
aH=111.41014794  
dH=60.46030143  
da=180.

--- Geometry Optimization ---

1\1\GINC-PAULING\Freq\RM062X\6-311++G(3df,2p)\H4O1Si1\ROSMUS\24-Jul-  
2012\1\#\#p m062x 6-311++G(3df,2p) opt=(call,z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Si,1,rS\H,1,rO,2,aO\H,2,ra,1,aa,3,da,0\H,2,rH,1,aH,3,dH,0\H,2,rH,1,aH,  
3,-  
dH,0\rS=1.64753915\rO=0.95620541\ra=1.4708587\rH=1.47774506\aO=119.08623721\  
aa=105.99841362\aH=111.41014794\dH=60.46030143\da=180.\Version=IA64L-  
G09RevA.02\State=1-A\HF=-367.1384346\RMSD=1.937e-09\RMSF=9.365e-  
05\ZeroPoint=0.0388095\Thermal=0.0427052\Dipole=0.5189897,0.,-  
0.003636\DipoleDeriv=-0.5434756,0.,0.0475692,0.,-0.669028,0.,0.0761532,0.,-  
1.3774078,1.1203739,0.,0.0027835,0.,1.1676777,0.,-  
0.0612371,0.,1.7467556,0.2225724,0.,-0.0307115,0.,0.3338369,0.,-  
0.0054872,0.,0.3669102,-0.2798412,0.,0.0183586,0.,-0.2314102,0.,-0.0232349,0.,-  
0.2231223,-0.2598148,-0.0334325,-0.0189999,-0.0341119,-0.3005382,-

```

0.0334575,0.006903,-0.0099831,-0.2565679,-0.2598148,0.0334325,-
0.0189999,0.0341119,-0.3005382,0.0334575,0.006903,0.0099831,-
0.2565679\Polar=31.4917459,0.,30.9634353,-0.3421033,0.,31.8990045\PG=CS
[SG(H2O1Si1),X(H2)]\NImag=0\0.46331382,0.,0.02620794,-
0.24457469,0.,0.46098086,-0.04731009,0.,-0.00513256,0.34476377,0.,-
0.03626207,0.,0.,0.31919720,0.02338137,0.,-0.28260199,-0.00754530,0.,0.42546488,-
0.42891979,0.,0.24934081,-0.00167382,0.,-0.00891010,0.43008452,0.,-
0.00208609,0.,0.,0.00111394,0.,0.,0.00097090,0.21822301,0.,-
0.14628011,0.02277485,0.,-0.01855574,-
0.23820994,0.,0.16447860,0.00140821,0.,0.00263204,-
0.16994002,0.,0.03941417,0.00112168,0.,-0.00068461,0.17678867,0.,0.00322345,0.,0.,-
0.02994556,0.,0.,0.00091122,0.,0.,0.02128375,0.01744344,0.,-
0.00979613,0.03246815,0.,-0.03335389,-0.00002991,0.,-0.00236711,-
0.04340792,0.,0.03662558,0.00575392,-0.00002289,-0.00113280,-0.06291993,-
0.05395487,-0.02317007,-0.00030629,-0.00040903,-0.00105165,-0.00468927,-
0.01144548,-0.00323688,0.05639105,-0.00035312,0.00445838,-0.00231490,-
0.05417246,-0.12705176,-0.04109949,-0.00015762,-0.00045499,0.00001552,-
0.00075945,0.00226357,-0.00028610,0.06063745,0.12970336,-0.00723656,-
0.01341368,-0.01115131,-0.02128256,-0.03793650,-0.04547663,-
0.00109543,0.00041540,0.00136217,0.00102316,0.00175104,0.00444577,0.02769768,0.
04643436,0.04561323,0.00575392,0.00002289,-0.00113280,-0.06291993,0.05395487,-
0.02317007,-0.00030629,0.00040903,-0.00105165,-0.00468927,0.01144548,-
0.00323687,0.00577052,-
0.00519481,0.00089372,0.05639105,0.00035312,0.00445838,0.00231490,0.05417246,-
0.12705176,0.04109949,0.00015762,-0.00045499,-
0.00001552,0.00075945,0.00226357,0.00028610,0.00519481,-0.00891857,0.00274939,-
0.06063745,0.12970336,-0.00723656,0.01341368,-0.01115131,-
0.02128256,0.03793650,-0.04547663,-0.00109543,-
0.00041540,0.00136217,0.00102316,-0.00175104,0.00444577,0.00089372,-
0.00274939,0.00520678,0.02769768,-0.04643436,0.04561323\|-0.00026358,0.,-
0.00002411,0.00028829,0.,0.00003164,0.00002457,0.,0.00000467,-
0.00002666,0.,0.00002112,-0.00001131,-0.00002338,-0.00001666,-
0.00001131,0.00002338,-0.00001666\|\|@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H4O1Si1\ROSMUS\24-Jul-2012\0\#p hf/cc-
pvqz scf=verytight pop=(nboread) geom=allcheck
guess=read\title\0,1\O\Si,1,1.6475391495\H,1,0.9562054141,2,119.08623721\H,2,1.47
08587022,1,105.99841362,3,180.,0\H,2,1.477745063,1,111.41014794,3,60.46030143,0\
H,2,1.477745063,1,111.41014794,3,-60.46030143,0\Version=IA64L-
G09RevA.02\State=1-A\HF=-366.2201945\RMSD=8.439e-
09\Dipole=0.5449412,0.,0.0016323\Quadrupole=0.5918154,-0.776962,0.1851466,0.,-
2.2345049,0.\PG=CS [SG(H2O1Si1),X(H2)]\|\|@

```

HF=-367.1384346

Sum of electronic and zero-point Energies= -367.099625

Sum of electronic and thermal Energies= -367.095729  
Sum of electronic and thermal Enthalpies= -367.094785  
Sum of electronic and thermal Free Energies= -367.124141  
NImag=0

#### Br2O1

-----  
0,1  
O  
Br,1,r2  
Br,1,r3,2,a3

r2=1.82016727  
r3=1.82016906  
a3=113.94311402

#### --- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Br2O1\ROSMUS\14-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Br,1,r2\Br,1,r3,2,a3\r2=1.82016727\r3=1.82016906\ a3=113.94311402\Version=IA64L-G09RevA.02\State=1-A\HF=-5223.458008\RMSD=2.812e-09\RMSF=4.147e-05\Dipole=0.2772612,0.,0.1802509\Quadrupole=-0.0036211,-1.6051268,1.6087479,0.,-1.8155742,0.\PG=CS [SG(Br2O1)]\@\

#### --- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br2O1\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\O\Br,1,1.82016727\Br,1,1.8201690561,2,113.94311399\Version=IA64L-G09RevA.02\State=1-A\HF=-5219.7066953\RMSD=3.313e-09\Dipole=0.3416296,0.,0.2220966\Quadrupole=-0.0712505,-1.5757567,1.6470072,0.,-1.9348081,0.\PG=CS [SG(Br2O1)]\@\

HF=-5223.458008

Sum of electronic and zero-point Energies= -5223.454626  
Sum of electronic and thermal Energies= -5223.450951  
Sum of electronic and thermal Enthalpies= -5223.450007  
Sum of electronic and thermal Free Energies= -5223.483407  
NImag=0

#### C2H6O1

-----  
0,1  
O  
C,1,r2



C,1,r3,2,a3  
X,1,1.,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0

r2=1.4014  
r3=1.4014  
a3=111.9711  
r5=1.0964  
r6=1.0875  
r7=1.0964  
a5=111.1641  
a6=107.8293  
a7=111.1449  
d5=206.2285  
d6=86.6772  
d7=327.129  
r8=1.0875  
r9=1.0964  
r10=1.0964  
a8=107.8271  
a9=111.1638  
a10=111.1476  
d8=179.9785  
d9=60.4263  
d10=-60.4762  
a4=95.577  
d4=266.6448

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C2H6O1\ROSMUS\14-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\C,1,r2\C,1,r3,2,a3\X,1,1.,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=1.4014\r3=1.4014\a3=111.9711\r5=1.0964\r6=1.0875\r7=1.0964\a5=111.1641\a6=107.8293\a7=111.1449\d5=206.2285\d6=86.6772\d7=327.129\r8=1.0875\r9=1.0964\r10=1.0964\a8=107.8271\a9=111.1638\a10=111.1476\d8=179.9785\d9=60.4263\d10=-60.4762\a4=95.577\d4=266.6448\\Version=IA64L-G09RevA.02\State=1-A\HF=-155.0066261\RMSD=2.541e-09\RMSF=1.979e-05\Dipole=0.4288834,-0.0000792,0.2894455\Quadrupole=-0.3595973,-0.3925009,0.7520983,-0.0001245,-1.3778281,-0.0002143\PG=C01 [X(C2H6O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C2H6O1\ROSMUS\18-Dec-2012\0\#p hf cc-  
 pvqz scf=verytight guess=read geom=allcheck  
 pop=savenbos\title\0,1\O\C,1,1.4014,C,1,1.4014,2,111.9711\X,1,1.,2,95.577,3,266.644  
 8,0\H,2,1.0964,1,111.1641,4,206.2285,0\H,2,1.0875,1,107.8293,4,86.6772,0\H,2,1.0964,  
 1,111.1449,4,327.129,0\H,3,1.0875,1,107.8271,2,179.9785,0\H,3,1.0964,1,111.1638,2,60  
 .4263,0\H,3,1.0964,1,111.1476,2,-60.4762,0\Version=IA64L-G09RevA.02\State=1-  
 A\HF=-154.138109\RMSD=9.006e-09\Dipole=0.4597362,-  
 0.00009,0.3102663\Quadrupole=-0.3598543,-0.3742754,0.7341297,-0.0001053,-  
 1.3558881,-0.000201\PG=C01 [X(C2H6O1)]\@

HF=-155.0066261

Sum of electronic and zero-point Energies= -154.925991  
 Sum of electronic and thermal Energies= -154.921741  
 Sum of electronic and thermal Enthalpies= -154.920797  
 Sum of electronic and thermal Free Energies= -154.951291  
 NImag=0

Cl2O1

-----  
 0,1  
 O  
 Cl,1,r2  
 Cl,1,r3,2,a3

r2=1.67613607  
 r3=1.67613726  
 a3=112.22346449

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Cl2O1\ROSMUS\14-Dec-  
 2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
 freq\title\0,1\O\Cl,1,r2\Cl,1,r3,2,a3\r2=1.67613607\r3=1.67613726\a3=112.22346449\|  
 Version=IA64L-G09RevA.02\State=1-A\HF=-995.491792\RMSD=9.735e-  
 09\RMSF=1.574e-06\Dipole=0.1897835,0.,0.1274729\Quadrupole=0.0976147,-  
 1.1359496,1.0383349,0.,-1.1512378,0.\PG=CS [SG(Cl2O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl2O1\ROSMUS\18-Dec-2012\0\#p hf cc-  
 pvqz scf=verytight guess=read geom=allcheck  
 pop=savenbos\title\0,1\O\Cl,1,1.67613607\Cl,1,1.6761372576,2,112.22346452\|Vers  
 ion=IA64L-G09RevA.02\State=1-A\HF=-993.7947757\RMSD=3.098e-  
 09\Dipole=0.2336002,0.,0.156903\Quadrupole=0.0543303,-1.0896571,1.0353268,0.,-  
 1.2005271,0.\PG=CS [SG(Cl2O1)]\@

HF=-995.491792

Sum of electronic and zero-point Energies= -995.487696  
Sum of electronic and thermal Energies= -995.484263  
Sum of electronic and thermal Enthalpies= -995.483319  
Sum of electronic and thermal Free Energies= -995.514197  
NImag=0

## F2O1

-----  
0,1  
O  
F,1,r2  
F,1,r3,2,a3

r2=1.36915137  
r3=1.36915257  
a3=103.07476509

### --- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\F2O1\ROSMUS\14-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\title\\0,1\O\F,1,r2\F,1,r3,2,a3\r2=1.36915137\r3=1.36915257\a3=103.07476509\\Version=IA64L-G09RevA.02\State=1-A\HF=-274.6588064\RMSD=6.926e-09\RMSF=6.133e-05\Dipole=-0.0836819,0.,-0.0664728\Quadrupole=0.1187411,-0.1920391,0.073298,0.,0.0978341,0.\PG=CS [SG(F2O1)]\@

### --- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F2O1\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\\title\\0,1\O\F,1,1.3691513703\F,1,1.3691525721,2,103.07476508\\Version=IA64L-G09RevA.02\State=1-A\HF=-273.5863678\RMSD=5.998e-09\Dipole=-0.1134039,0.,-0.0900831\Quadrupole=0.0681077,-0.048846,-0.0192617,0.,0.1880983,0.\PG=CS [SG(F2O1)]\@

HF=-274.6588064

Sum of electronic and zero-point Energies= -274.652695  
Sum of electronic and thermal Energies= -274.649607  
Sum of electronic and thermal Enthalpies= -274.648663  
Sum of electronic and thermal Free Energies= -274.677149  
NImag=0

## Ge2H6O1

-----  
0,1

O

Ge,1,r2

Ge,1,r3,2,a3

X,1,r4,2,a4,3,d4,0

H,2,r5,1,a5,4,d5,0

H,2,r6,1,a6,4,d6,0

H,2,r7,1,a7,4,d7,0

H,3,r8,1,a8,2,d8,0

H,3,r9,1,a9,2,d9,0

H,3,r10,1,a10,2,d10,0

r2=1.77539471

r3=1.77539963

a3=130.03694186

r5=1.54544301

r6=1.53699158

r7=1.54544321

a5=108.95409957

a6=106.54677402

a7=108.95394641

d5=206.73812293

d6=86.62360435

d7=326.50979358

r8=1.53699372

r9=1.54543419

r10=1.54543586

a8=106.54667411

a9=108.95329306

a10=108.95270805

d8=180.02620619

d9=59.91251644

d10=-59.86113456

r4=1.

a4=95.577

d4=266.6448

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Ge2H6O1\ROSMUS\14-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Ge,1,r2\Ge,1,r3,2,a3\X,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=1.77539471\r3=1.77539963\a3=130.03694186\r5=1.54544301\r6=1.53699158\r7=1.54544321\a5=108.95409957\a6=106.54677402\a7=108.95394641\d5=206.73812293\d6=86.62360435\d7=326.50979358\r8=1.53699372\r9=1.54543419\r10=1.54543586\a8=106.54667411\a9=108.95329306\a10=108.95270805\d8=180.02620619\d9=59.91251644\d10=-59.86113456\r4=1.\a4=95.577\d4=266.6448\Version=IA64L-G09RevA.02\State=1-

A\HF=-4232.7950794\RMSD=2.598e-09\RMSF=7.919e-  
 05\Dipole=0.2965247,0.0000055,0.1381209\Quadrupole=-0.8203728,-  
 0.7536199,1.5739927,-0.0000566,-1.4250613,-0.0000238\PG=C01 [X(Ge2H6O1)]\@  
 --- NBO Single Point ---  
 1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge2H6O1\ROSMUS\18-Dec-2012\0\#p hf  
 cc-pvqz scf=verytight guess=read geom=allcheck  
 pop=savenbos\title\0,1\O\Ge,1,1.7753947167\Ge,1,1.7753996375,2,130.03693401\X,1,  
 1.,2,95.577,3,266.6448,0\H,2,1.5454430002,1,108.95409963,4,206.73812298,0\H,2,1.53  
 69915892,1,106.54677242,4,86.62360438,0\H,2,1.5454431991,1,108.95394641,4,326.50  
 97936,0\H,3,1.5369937293,1,106.54667249,2,180.02620615,0\H,3,1.5454341746,1,108.  
 95329312,2,59.91251637,0\H,3,1.5454358475,1,108.95270805,2,-  
 59.86113461,0\Version=IA64L-G09RevA.02\State=1-A\HF=-  
 4229.2423801\RMSD=4.168e-  
 09\Dipole=0.3309564,0.0000039,0.1541617\Quadrupole=-0.8544276,-  
 0.67802,1.5324475,-0.0000388,-1.4206211,-0.0000145\PG=C01 [X(Ge2H6O1)]\@

HF=-4232.7950794

Sum of electronic and zero-point Energies=	-4232.743815
Sum of electronic and thermal Energies=	-4232.737513
Sum of electronic and thermal Enthalpies=	-4232.736569
Sum of electronic and thermal Free Energies=	-4232.775674
NImag=0	

## H2O3

-----  
 0,1  
 O  
 O,1,r2  
 O,1,r3,2,a3  
 X,1,r4,2,a4,3,d4,0  
 H,2,r5,1,a5,4,d5,0  
 H,3,r6,1,a6,2,d6,0

r2=1.39608124  
 r3=1.39591533  
 r5=0.96594198  
 r6=0.9659482  
 a3=107.35364818  
 a5=103.1368394  
 a6=103.14762872  
 d5=200.64716833  
 d6=266.05759736  
 r4=1.  
 a4=101.913

d4=106.634

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H2O3\ROSMUS\14-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\O,1,r2\O,1,r3,2,a3\X,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\|r2=1.39608124|r3=1.39591533|r5=0.96594198|r6=0.9659482|a3=107.35364818|a5=103.1368394|a6=103.14762872\d5=200.64716833\d6=266.05759736|r4=1.|a4=101.913\d4=106.634\Version=IA64L-G09RevA.02\State=1-A\HF=-226.6847501\RMSD=4.062e-09\RMSF=1.869e-04\Dipole=0.1548598,1.2484696,0.1141826\Quadrupole=-0.9099116,1.2848521,-0.3749405,0.7447006,-0.861634,0.5485236\PG=C01 [X(H2O3)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H2O3\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\O\O,1,1.3960812393\O,1,1.3959153296,2,107.35364818\X,1,1.,2,101.913,3,106.634,0\H,2,0.9659419756,1,103.1368394,4,200.64716833,0\H,3,0.9659482022,1,103.14762872,2,266.05759736,0\Version=IA64L-G09RevA.02\State=1-A\HF=-225.6497664\RMSD=6.096e-09\Dipole=0.165351,1.3082988,0.1219471\Quadrupole=-0.9492259,1.3743356,-0.4251096,0.7632875,-0.844393,0.5621728\PG=C01 [X(H2O3)]\@

HF=-226.6847501

Sum of electronic and zero-point Energies=	-226.653259
Sum of electronic and thermal Energies=	-226.649479
Sum of electronic and thermal Enthalpies=	-226.648535
Sum of electronic and thermal Free Energies=	-226.678050
NImag=	0

H2O1S2

-----  
0,1  
O  
S,1,r2  
S,1,r3,2,a3  
X,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.66506028  
r3=1.66506887  
r5=1.34301533  
r6=1.34301387  
a3=118.4758315

a5=97.18216497  
a6=97.18087552  
d5=297.43168224  
d6=275.45288981  
r4=1.  
a4=114.82  
d4=212.888

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H2O1S2\ROSMUS\14-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\S,1,r2\S,1,r3,2,a3\X,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\r2=1.66506028\r3=1.66506887\r5=1.34301533\r6=1.34301387\a3=118.4758315\a5=97.18216497\a6=97.18087552\d5=297.43168224\d6=275.45288981\r4=1.\a4=114.82\d4=212.888\Version=IA64L-G09RevA.02\State=1-A\HF=-872.7405166\RMSD=4.980e-09\RMSF=7.927e-05\Dipole=0.3096862,0.6075843,0.1843101\Quadrupole=-1.7638453,1.8777876,-0.1139423,0.7879974,-1.520807,0.4689781\PG=C01  
[X(H2O1S2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H2O1S2\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\O\S,1,1.6650602829\S,1,1.6650688737,2,118.47583098\X,1,1.,2,114.82,3,212.888,0\H,2,1.3430153256,1,97.18216501,4,297.43167503,0\H,3,1.3430138716,1,97.18087554,2,275.45289598,0\Version=IA64L-G09RevA.02\State=1-A\HF=-871.1010602\RMSD=4.689e-09\Dipole=0.3685332,0.6649637,0.219331\Quadrupole=-1.8004782,1.9337449,-0.1332666,0.8369977,-1.5367539,0.4981395\PG=C01  
[X(H2O1S2)]\@

HF=-872.7405166

Sum of electronic and zero-point Energies=	-872.718681
Sum of electronic and thermal Energies=	-872.714166
Sum of electronic and thermal Enthalpies=	-872.713222
Sum of electronic and thermal Free Energies=	-872.745935
NImag=	0

H2O1Se2

-----  
0,1  
O  
Se,1,r2  
Se,1,r3,2,a3  
X,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.80628536  
r3=1.80628538  
r5=1.47369269  
r6=1.47369281  
a3=119.87410778  
a5=95.67995558  
a6=95.68002164  
d5=217.43720367  
d6=275.18331421  
r4=1.  
a4=111.093  
d4=132.62

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H2O1Se2\ROSMUS\14-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Se,1,r2\Se,1,r3,2,a3\X,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\r2=1.80628536\r3=1.80628538\r5=1.47369269\r6=1.47369281\a3=119.87410778\a5=95.67995558\a6=95.68002164\d5=217.43720367\d6=275.18331421\r4=1.\a4=111.093\d4=132.62\Version=IA64L-G09RevA.02\State=1-A\HF=-4879.4736991\RMSD=5.080e-09\RMSF=1.428e-04\Dipole=0.3904404,0.4445504,0.2259945\Quadrupole=-2.2238608,1.828246,0.3956148,0.7076798,-2.2801,0.4096289\PG=C01[X(H2O1Se2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H2O1Se2\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\O\Se,1,1.8062853575\Se,1,1.8062853824,2,119.87410779\X,1,1.,2,111.093,3,132.62,0\H,2,1.4736926901,1,95.67995559,4,217.43720377,0\H,3,1.473692814,1,95.68002165,2,275.18331414,0\Version=IA64L-G09RevA.02\State=1-A\HF=-4875.7828033\RMSD=3.025e-09\Dipole=0.4544203,0.4793098,0.2630271\Quadrupole=-2.2764823,1.914349,0.3621333,0.7493339,-2.2967609,0.4337398\PG=C01[X(H2O1Se2)]\@

HF=-4879.4736991

Sum of electronic and zero-point Energies= -4879.453848  
Sum of electronic and thermal Energies= -4879.449135  
Sum of electronic and thermal Enthalpies= -4879.448191  
Sum of electronic and thermal Free Energies= -4879.483421  
NImag=0

H6O1Si2



-----  
0,1  
O  
Si,1,r2  
Si,1,r3,2,a3  
X,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0

r2=1.63481999  
r3=1.63484627  
a3=144.604143  
r5=1.47788317  
r6=1.47346884  
r7=1.47487002  
a5=109.8288352  
a6=108.88086959  
a7=109.7855921  
d5=246.01376963  
d6=125.96317641  
d7=366.12134206  
r8=1.4727188  
r9=1.47762583  
r10=1.47553293  
a8=108.71738627  
a9=109.82447789  
a10=109.94986932  
d8=146.64125411  
d9=26.60579795  
d10=-93.52910441

r4=1.  
a4=95.577  
d4=266.6448

--- Geometry Optimization ---

1\1\GINC-PAULING\Freq\RM062X\6-311++G(3df,2p)\H6O1Si2\ROSMUS\17-Dec-2012\1\1\#p m062x 6-311++G(3df,2p) opt=(calcall,z-matrix,noeigen) optcyc=100  
freq\title\0,1\O\Si,1,r2\Si,1,r3,2,a3\X,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=1.63481999\r3=1.63484627\a3=144.604143\r5=1.47788317\r6=1.47346884\r7=1.47487002\a5=109.8288352\a6=108.88086959\a7=109.7855921\d5=246.01376963\d6=125.96317

641\d7=366.12134206\r8=1.4727188\r9=1.47762583\r10=1.47553293\ a8=108.71738627  
\ a9=109.82447789\ a10=109.94986932\d8=146.64125411\d9=26.60579795\d10=-  
93.52910441\r4=1.\ a4=95.577\d4=266.6448\\Version=IA64L-G09RevA.02\State=1-  
A\HF=-657.8585242\RMSD=2.121e-09\RMSF=2.062e-  
05\ZeroPoint=0.055461\Thermal=0.0606144\Dipole=0.1249997,-  
0.0020685,0.0400736\DipoleDeriv=-0.8826575,0.0136823,0.5316866,0.0185852,-  
0.6064287,0.0071462,0.5328618,0.0049471,-2.3852924,1.1082306,-0.0121773,-  
0.043506,-0.0114023,1.0914337,0.0035036,-0.2508086,0.005229,2.1374526,1.3113385,-  
0.0083471,-0.5395422,-0.006055,1.0915713,-0.0089024,-0.3326653,-  
0.0107606,1.9337675,-0.2852574,0.0220186,-0.0312156,0.0206214,-  
0.2393931,0.0128071,0.0316433,-0.0038103,-0.2874404,-0.2680583,-  
0.0310036,0.0381648,-0.0323971,-0.2512798,0.0234219,0.0183186,-0.0040266,-  
0.2612756,-0.2322201,0.0119549,0.0173749,0.0147265,-0.2976031,-  
0.0435327,0.0265011,0.0033168,-0.2766945,-0.2449298,-0.0233577,-0.0267874,-  
0.0140861,-0.2485893,-0.0366306,-0.0049654,-0.0136426,-0.2923009,-  
0.2791991,0.0232242,0.034298,0.0304935,-0.2421008,0.0050045,-  
0.0290934,0.0207328,-0.2823978,-0.227247,0.0040057,0.0195269,-0.0204861,-  
0.2976102,0.0371823,0.0082079,-0.0019856,-  
0.2858186\Polar=52.3926644,0.1048806,52.2017272,-  
2.5325621,0.0276012,59.649015\PG=C01 [X(H6O1Si2)]\NImag=1\\0.14377539,-  
0.00300623,0.04148997,-0.14665321,-0.00096256,0.55584785,-  
0.03711594,0.00097644,0.00137375,0.33158222,0.00105296,-  
0.03484839,0.00033367,0.00276285,0.32820406,0.00383873,0.00047077,-0.28242471,-  
0.01138699,0.00193940,0.42987726,-0.11713242,0.00099224,0.11641521,-0.00019360,-  
0.00109455,0.01598986,0.35353088,0.00089953,-0.03482676,0.00037258,-  
0.00090964,0.00051399,-0.00066330,0.00289672,0.32800263,0.11386718,0.00014580,-  
0.20239880,0.01126604,-0.00011114,-0.03884930,-0.04082598,-  
0.00043673,0.41073912,0.00503995,0.00039807,-0.00402186,-0.14515634,0.04237423,-  
0.04108420,-  
0.00200930,0.00018435,0.00066300,0.14918554,0.00025851,0.00512800,0.00129651,0.  
04244927,-0.04790456,0.01620738,0.00051460,-0.00055960,-0.00043383,-  
0.04771181,0.04039178,-0.01205631,0.00555207,-0.01471953,-  
0.03765495,0.01478956,-0.04246897,-0.00430833,0.00015565,0.00518811,0.04803783,-  
0.01843714,0.04385875,0.00350194,-0.00043439,0.00272647,-0.11119146,-  
0.06598600,0.03370844,0.00022410,-0.00015502,-0.00136092,-0.00801888,-  
0.00750025,0.00233356,0.11122765,-0.00076318,0.00462042,0.00224881,-0.06604148,-  
0.08510567,0.02740109,0.00051447,-0.00040700,-0.00080538,0.00307958,0.00537308,-  
0.00061649,0.07347944,0.08209511,0.01318592,0.00811783,-  
0.01442124,0.02965847,0.02477197,-0.03781342,-0.00222052,0.00133404,0.00302751,-  
0.00232181,-0.00152670,0.00452262,-0.03776849,-  
0.03076468,0.04145720,0.00490472,0.00058676,0.00055607,-  
0.03517681,0.02071875,0.00808965,-0.00026839,0.00002865,-0.00060090,-  
0.00001298,0.01224160,0.00243736,0.00403114,-0.01006414,-  
0.00176921,0.02616851,0.00096336,0.00444697,-0.00347534,0.02068767,-0.15914408,-  
0.04556922,-0.00088554,-0.00079421,0.00120338,0.00177504,-0.00273390,-  
0.00128627,0.00064344,-0.00689386,-0.00186056,-

0.02344667,0.16473846,0.00517708,-0.01376904,-0.01457412,0.00701849,-  
0.04160726,-0.04106819,-0.00367159,-0.00123230,0.00383588,-  
0.00081915,0.00267269,0.00464600,-0.00007456,0.00234773,0.00467819,-  
0.00889359,0.05144281,0.04393594,0.00536677,0.00375797,0.01118004,-  
0.00047599,0.00055559,-0.00101867,-0.06333645,-0.03801201,-  
0.05563131,0.00028728,-0.00008767,0.00034119,0.00007959,-  
0.00005257,0.00014266,0.00009727,0.00006395,0.00043616,0.05941056,0.00071111,0.  
00466202,-0.00205557,-0.00005609,-0.00034458,0.00088605,-0.03667814,-  
0.07246831,-0.05583971,-0.00006475,0.00011461,-  
0.00013860,0.00001454,0.00010568,-0.00011657,-0.00002800,0.00009355,-  
0.00000815,0.04074741,0.06808514,0.00009952,-0.00595265,-0.01652132,-  
0.00034928,-0.00107169,0.00371220,-0.05129026,-0.05414520,-0.10257286,-  
0.00013838,0.00009334,-0.00051202,0.00014720,0.00010881,-0.00034037,0.00009868,-  
0.00016509,-0.00083019,0.05449755,0.06240156,0.11176022,-  
0.00881690,0.00434099,0.00813112,-0.00126891,0.00033762,-0.00519169,-  
0.13793093,0.05235921,-0.03028694,0.00039136,-0.00012448,0.00052203,0.00010861,-  
0.00012748,0.00052032,0.00016595,0.00008722,0.00057703,-0.00413662,0.00313355,-  
0.00363892,0.14826636,0.00114959,0.00489809,-0.00115045,0.00020342,-  
0.00056152,0.00077862,0.05344495,-0.05726789,0.01420272,-0.00005240,0.00007209,-  
0.00015859,-0.00001936,0.00012188,-0.00012934,-0.00001708,0.00010729,-  
0.00005798,-0.00564263,0.00567952,-0.00245167,-  
0.06023554,0.05095552,0.01556802,-0.00543292,-0.00088550,-  
0.00023003,0.00000362,0.00445327,-0.03352548,0.01565648,-0.03797283,-  
0.00020967,0.00008447,-0.00006639,0.00012152,0.00006189,-0.00029557,0.00005107,-  
0.00010781,-0.00034698,-0.00837679,0.00336356,0.00025855,0.02986128,-  
0.01567556,0.03204353,0.00047649,-0.00761185,0.01029240,-0.00100317,-  
0.00072144,-0.00294512,-0.03288389,-0.01729180,0.00290981,0.00029337,-  
0.00003977,0.00034762,0.00003731,-  
0.00002464,0.00057266,0.00009061,0.00011153,0.00025013,0.00270759,-  
0.00777963,0.00057389,0.00322106,0.01116906,-0.00325993,0.02706064,-  
0.00126565,0.00442967,0.00339235,-0.00007243,-0.00080925,-0.00145079,-  
0.01970476,-0.16219285,0.04207489,0.00001769,0.00011850,0.00013982,-  
0.00004240,0.00009036,0.00017401,-0.00001988,0.00017977,0.00021151,-0.00133002,-  
0.00592764,0.00118260,0.00022891,-  
0.00400498,0.00204628,0.02218855,0.16811642,0.00697307,0.01183071,-  
0.00990263,0.00030449,0.00095186,0.00458186,0.00343710,0.03895878,-0.04099683,-  
0.00010577,0.00004328,-0.00044857,0.00016677,0.00001822,-0.00081492,0.00003087,-  
0.00018188,-0.00027652,-0.00157083,-0.00849257,0.00504578,-  
0.00049423,0.00464225,0.00281192,-0.00874147,-  
0.04777065,0.03999991\\0.00004215,-0.00006614,-0.00000215,-  
0.00004168,0.00000749,0.00000034,-  
0.00000160,0.00005917,0.00000216,0.00000051,0.00000092,0.00000027,0.00000080,-  
0.00000005,-0.00000033,-0.00000049,0.00000014,-0.00000021,0.00000229,-  
0.00000068,0.00000232,-0.00000145,0.00000087,-0.00000016,-0.00000053,-  
0.00000173,-0.00000224\\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H6O1Si2\ROSMUS\18-Dec-2012\0\# hf cc-  
pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\O\Si,1,1.634819994\Si,1,1.6348462714,2,144.60414327\X,1,1.,  
2,95.577,3,266.6448,0\H,2,1.4778831741,1,109.82883535,4,246.01377847,0\H,2,1.4734  
688393,1,108.88086973,4,125.96318543,0\H,2,1.4748700248,1,109.78559184,4,366.121  
35103,0\H,3,1.4727188006,1,108.71738625,2,146.64125491,0\H,3,1.4776258267,1,109.  
82447793,2,26.60579872,0\H,3,1.4755329342,1,109.9498693,2,-  
93.52910364,0\Version=IA64L-G09RevA.02\State=1-A\HF=-  
656.3837075\RMSD=2.697e-09\Dipole=0.1396563,-0.0015163,0.0449444\Quadrupole=-  
0.4544014,-0.2532091,0.7076105,0.0161206,-0.4080746,0.0090037\PG=C01  
[X(H6O1Si2)]\@

HF=-657.8585242

Sum of electronic and zero-point Energies=	-657.803063
Sum of electronic and thermal Energies=	-657.797910
Sum of electronic and thermal Enthalpies=	-657.796966
Sum of electronic and thermal Free Energies=	-657.831754

NImag=1

Br1H2P1

-----  
0,1  
P  
C,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.85415742  
r3=1.41187092  
r4=1.41188126  
a3=97.63669255  
a4=97.62305008  
d4=94.37069899  
r5=1.0865133  
r6=1.08860032  
r7=1.08859218  
a5=113.45097385  
a6=108.61230214  
a7=108.62322647  
d5=47.35049076  
d6=-74.1830529

d7=168.90217158

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C1H5P1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\PC,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.85415742\r3=1.41187092\r4=1.41188126\a3=97.63669255\a4=97.62305008\d4=94.37069899\r5=1.0865133\r6=1.08860032\r7=1.08859218\a5=113.45097385\a6=108.61230214\a7=108.62322647\d5=47.35049076\d6=-74.1830529\d7=168.90217158\Version=IA64L-G09RevA.02\State=1-A\HF=-382.4329916\RMSD=7.477e-09\RMSF=3.987e-05\Dipole=0.1495254,-0.1613505,0.4001233\Quadrupole=0.1957111,0.1087709,-0.304482,0.5710984,-0.6938982,0.7482216\PG=C01 [X(C1H5P1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br1H2P1\ROSMUS\26-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\P\Br,1,2.2362958807\H,1,1.4123778313,2,95.78186816\H,1,1.4123778313,2,95.78186816,3,92.94544978,0\Version=IA64L-G09RevA.02\State=1-A\HF=-2914.4020477\RMSD=4.271e-09\Dipole=0.2175689,-0.2290514,-0.6101751\Quadrupole=-0.5493519,-0.6101864,1.1595383,0.5911644,-1.0067664,1.0598995\PG=CS [SG(Br1P1),X(H2)]\@

HF=-2916.725074

Sum of electronic and zero-point Energies= -2916.706600  
Sum of electronic and thermal Energies= -2916.703303  
Sum of electronic and thermal Enthalpies= -2916.702359  
Sum of electronic and thermal Free Energies= -2916.732694  
NImag=0

C1H5P1

-----  
0,1  
P  
C,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.85415742  
r3=1.41187092  
r4=1.41188126  
a3=97.63669255

a4=97.62305008  
d4=94.37069899  
r5=1.0865133  
r6=1.08860032  
r7=1.08859218  
a5=113.45097385  
a6=108.61230214  
a7=108.62322647  
d5=47.35049076  
d6=-74.1830529  
d7=168.90217158

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C1H5P1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\PC,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.85415742\r3=1.41187092\r4=1.41188126\a3=97.63669255\a4=97.62305008\d4=94.37069899\r5=1.0865133\r6=1.08860032\r7=1.08859218\a5=113.45097385\a6=108.61230214\a7=108.62322647\d5=47.35049076\d6=-74.1830529\d7=168.90217158\\Version=IA64L-G09RevA.02\State=1-A\HF=-382.4329916\RMSD=7.477e-09\RMSF=3.987e-05\Dipole=0.1495254,-0.1613505,0.4001233\Quadrupole=0.1957111,0.1087709,-0.304482,0.5710984,-0.6938982,0.7482216\PG=C01 [X(C1H5P1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C1H5P1\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\PC,1,1.8541574163\H,1,1.4118709214,2,97.63669255\H,1,1.4118812553,2,97.62305008,3,94.37069899,0\H,2,1.086513299,1,113.45097385,4,47.35049076,0\H,2,1.088600325,1,108.61230214,4,-74.1830529,0\H,2,1.088592181,1,108.62322647,4,168.90217158,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-381.5466304\RMSD=3.357e-09\Dipole=0.1655794,-0.1786374,0.4174331\Quadrupole=0.2298871,0.1318294,-0.3617165,0.6434141,-0.7569178,0.8163266\PG=C01 [X(C1H5P1)]\@\

HF=-382.4329916

Sum of electronic and zero-point Energies= -382.378197  
Sum of electronic and thermal Energies= -382.374421  
Sum of electronic and thermal Enthalpies= -382.373477  
Sum of electronic and thermal Free Energies= -382.402706  
NImag=0

C11H2P1

-----  
0,1

P  
Cl,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=2.06780419  
r3=1.41192632  
r4=1.41192632  
a3=96.4771215  
a4=96.4771215  
d4=93.1083215

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Cl1H2P1\ROSMUS\26-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Cl,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=2.06780419\r3=1.41192632\r4=1.41192632\a3=96.4771215\a4=96.4771215\d4=93.1083215\Version=IA64L-G09RevA.02\State=1-A\HF=-802.7508843\RMSD=3.296e-09\RMSF=2.353e-05\Dipole=0.1983529,-0.2094165,-0.5423248\Quadrupole=-0.1752417,-0.2336979,0.4089396,0.5382346,-0.7297283,0.7704304\PG=CS [SG(Cl1P1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl1H2P1\ROSMUS\26-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\P\Cl,1,2.0678041903\H,1,1.4119263193,2,96.4771215\H,1,1.4119263193,2,96.4771215,3,93.1083215,0\Version=IA64L-G09RevA.02\State=1-A\HF=-801.4582851\RMSD=3.057e-09\Dipole=0.2189537,-0.2311663,-0.5890535\Quadrupole=-0.0913708,-0.1581587,0.2495295,0.6149477,-0.8084363,0.8535285\PG=CS [SG(Cl1P1),X(H2)]\@

HF=-802.7508843

Sum of electronic and zero-point Energies=	-802.731976
Sum of electronic and thermal Energies=	-802.728788
Sum of electronic and thermal Enthalpies=	-802.727844
Sum of electronic and thermal Free Energies=	-802.756862
NImag=0	

F1H2P1

-----  
0,1  
P  
F,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.61082231  
r3=1.41635737  
r4=1.41635737  
a3=97.35403836  
a4=97.35403836  
d4=93.03463076

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\F1H2P1\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\F,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.61082231\r3=1.41635737\r4=1.41635737\a3=97.35403836\a4=97.35403836\d4=93.03463076\Version=IA64L-G09RevA.02\State=1-A\HF=-442.3947969\RMSD=4.660e-09\RMSF=2.332e-04\Dipole=0.1893717,-0.199677,-0.4808723\Quadrupole=0.3168258,0.2549064,-0.5717322,0.5839929,-0.5449629,0.5746188\PG=CS [SG(F1P1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F1H2P1\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\P\F,1,1.6108223087\H,1,1.4163573739,2,97.35403836\H,1,1.4163573739,2,97.35403836,3,93.03463076,0\Version=IA64L-G09RevA.02\State=1-A\HF=-441.4195224\RMSD=9.590e-09\Dipole=0.2071371,-0.2184091,-0.5414948\Quadrupole=0.3670304,0.297923,-0.6649534,0.6517859,-0.6152015,0.6486796\PG=CS [SG(F1P1),X(H2)]\@

HF=-442.3947969

Sum of electronic and zero-point Energies=	-442.374762
Sum of electronic and thermal Energies=	-442.371752
Sum of electronic and thermal Enthalpies=	-442.370808
Sum of electronic and thermal Free Energies=	-442.398437
NImag=0	

Ge1H5P1

-----

0,1  
P  
Ge,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=2.3330711  
r3=1.41286394



r4=1.4128827  
a3=93.40137159  
a4=93.30967935  
d4=93.44220854  
r5=1.54222537  
r6=1.54172536  
r7=1.54170187  
a5=112.37928579  
a6=108.0184034  
a7=108.11790758  
d5=47.70483861  
d6=-73.11919252  
d7=168.62749777

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Ge1H5P1\ROSMUS\26-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Ge,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=2.3330711\r3=1.41286394\r4=1.4128827\a3=93.40137159\a4=93.30967935\d4=93.44220854\r5=1.54222537\r6=1.54172536\r7=1.54170187\a5=112.37928579\a6=108.0184034\a7=108.11790758\d5=47.70483861\d6=-73.11919252\d7=168.62749777\Version=IA64L-G09RevA.02\State=1-A\HF=-2421.3030545\RMSD=6.715e-09\RMSF=3.382e-05\Dipole=0.1483539,-0.1558391,0.1516371\Quadrupole=0.4818597,0.4210999,-0.9029596,0.519074,-0.8173231,0.863167\PG=C01 [X(Ge1H5P1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge1H5P1\ROSMUS\26-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\P\Ge,1,2.3330710952\H,1,1.4128639366,2,93.40137159\H,1,1.4128827032,2,93.30967935,3,93.44220854,0\H,2,1.5422253746,1,112.37928579,4,47.70483861,0\H,2,1.5417253629,1,108.0184034,4,-73.11919252,0\H,2,1.5417018662,1,108.11790758,4,168.62749777,0\Version=IA64L-G09RevA.02\State=1-A\HF=-2419.0728796\RMSD=5.896e-09\Dipole=0.1710011,-0.1795487,0.1637881\Quadrupole=0.5650755,0.4979621,-1.0630377,0.566295,-0.9019208,0.9526947\PG=C01 [X(Ge1H5P1)]\@\

HF=-2421.3030545

Sum of electronic and zero-point Energies= -2421.262484  
Sum of electronic and thermal Energies= -2421.257587  
Sum of electronic and thermal Enthalpies= -2421.256643  
Sum of electronic and thermal Free Energies= -2421.290364  
NImag=0

H4N1P1

-----  
0,1  
P  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0

r2=1.70367039  
r4=1.41152529  
r5=1.00701011  
a4=98.78087673  
a5=114.70516235  
d4=95.05519339  
d5=200.50551009  
r6=1.00796314  
a6=120.39751933  
d6=62.83118798  
r3=1.41876593  
a3=103.15501073

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H4N1P1\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\PN,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\r2=1.70367039\r4=1.41152529\r5=1.00701011\ a4=98.78087673\ a5=114.70516235\ d4=95.05519339\ d5=200.50551009\ r6=1.00796314\ a6=120.39751933\ d6=62.83118798\ r3=1.41876593\ a3=103.15501073\ \Version=IA64L-G09RevA.02\State=1-A\HF=-398.4884893\RMSD=8.710e-09\RMSF=2.941e-05\Dipole=0.438383,0.0288666,0.4192766\Quadrupole=-0.8259219,0.118076,0.7078459,-0.420667,0.5313661,1.440961\PG=C01  
[X(H4N1P1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H4N1P1\ROSMUS\20-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\PN,1,1.7036703901\H,1,1.4187659279,2,103.15501073\H,1,1.4115252869,2,98.78087673,3,95.05519339,0\H,2,1.0070101063,1,114.70516235,4,200.50551009,0\H,2,1.007963141,1,120.39751933,4,62.83118798,0\ \Version=IA64L-G09RevA.02\State=1-A\HF=-397.5603657\RMSD=8.844e-09\Dipole=0.4683605,0.0226898,0.4291515\Quadrupole=-0.7923159,0.128994,0.6633219,-0.3120578,0.4768117,1.5282346\PG=C01  
[X(H4N1P1)]\@\

HF=-398.4884893

Sum of electronic and zero-point Energies= -398.444331  
Sum of electronic and thermal Energies= -398.440641  
Sum of electronic and thermal Enthalpies= -398.439697  
Sum of electronic and thermal Free Energies= -398.468495  
NImag=0

## H5P1Si1

-----  
0,1  
P  
Si,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=2.2554444  
r3=1.41310982  
r4=1.41310478  
a3=93.60095669  
a4=93.57633853  
d4=93.74475721  
r5=1.47675952  
r6=1.47612446  
r7=1.47617703  
a5=113.34377487  
a6=108.05174277  
a7=108.08073562  
d5=46.87086949  
d6=-74.16217023  
d7=167.9158686

### --- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H5P1Si1\ROSMUS\26-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Si,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=2.2554444\r3=1.41310982\r4=1.41310478\a3=93.60095669\a4=93.57633853\d4=93.74475721\r5=1.47675952\r6=1.47612446\r7=1.47617703\a5=113.34377487\a6=108.05174277\a7=108.08073562\d5=46.87086949\d6=-74.16217023\d7=167.9158686\Version=IA64L-G09RevA.02\State=1-A\HF=-633.8095047\RMSD=2.919e-09\RMSF=2.149e-05\Dipole=0.1521616,-0.1622812,0.1285362\Quadrupole=0.4064457,0.3380123,-0.744458,0.5255154,-0.7026968,0.7495186\PG=C01 [X(H5P1Si1)]\@\

### --- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H5P1Si1\ROSMUS\26-Jul-2012\0\#p hf/cc-  
 pvqz scf=verytight pop=(nboread) geom=allcheck  
 guess=read\title\0,1\P\Si,1,2.2554444047\H,1,1.413109816,2,93.60095669\H,1,1.41310  
 47791,2,93.57633853,3,93.74475721,0\H,2,1.4767595165,1,113.34377487,4,46.8708694  
 9,0\H,2,1.4761244557,1,108.05174277,4,-  
 74.16217023,0\H,2,1.4761770272,1,108.08073562,4,167.9158686,0\Version=IA64L-  
 G09RevA.02\State=1-A\HF=-632.6142009\RMSD=4.413e-09\Dipole=0.1743513,-  
 0.1859261,0.1566958\Quadrupole=0.4902617,0.4150491,-0.9053108,0.5776897,-  
 0.7688489,0.8200119\PG=C01 [X(H5P1Si1)]\@

HF=-633.8095047

Sum of electronic and zero-point Energies= -633.767281  
 Sum of electronic and thermal Energies= -633.762618  
 Sum of electronic and thermal Enthalpies= -633.761674  
 Sum of electronic and thermal Free Energies= -633.793745  
 NImag=0

Br2H1P1

-----  
 0,1  
 P  
 Br,1,r2  
 Br,1,r3,2,a3  
 H,1,r4,2,a4,3,d4,0  
  
 r2=2.22721566  
 r3=2.22753245  
 r4=1.40979618  
 a3=102.81389307  
 a4=94.13987138  
 d4=95.22291838

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Br2H1P1\ROSMUS\11-Dec-  
 2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
 freq\title\0,1\P\Br,1,r2\Br,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=2.22721566\r3=2.22753245\r  
 4=1.40979618\a3=102.81389307\a4=94.13987138\d4=95.22291838\Version=IA64L-  
 G09RevA.02\State=1-A\HF=-5490.3311819\RMSD=3.397e-09\RMSF=2.138e-  
 04\Dipole=-0.3244912,-0.23807,-0.258372\Quadrupole=0.3170064,-0.2109956,-  
 0.1060108,0.8759081,0.9290996,0.6986602\PG=C01 [X(Br2H1P1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br2H1P1\ROSMUS\18-Dec-2012\0\#p hf cc-  
 pvqz scf=verytight guess=read geom=allcheck  
 pop=savenbos\title\0,1\P\Br,1,2.2272156639\Br,1,2.2275324481,2,102.81389307\H,1,1

.4097961766,2,94.13987138,3,95.22291838,0\\Version=IA64L-G09RevA.02\\State=1-A\\HF=-5486.3118404\\RMSD=5.068e-09\\Dipole=-0.355151,-0.2804354,-0.2828322\\Quadrupole=0.2265523,0.036382,-0.2629342,1.00056,1.0752749,0.7981354\\PG=C01 [X(Br2H1P1)]\\@

HF=-5490.3311819

Sum of electronic and zero-point Energies= -5490.319641  
Sum of electronic and thermal Energies= -5490.315384  
Sum of electronic and thermal Enthalpies= -5490.314440  
Sum of electronic and thermal Free Energies= -5490.349962  
NImag=0

C2H7P1

-----  
0,1  
P  
C,1,r2  
C,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0

r2=1.84852576  
r3=1.84869811  
r4=1.41360179  
a3=99.17977244  
a4=96.93712075  
d4=98.18077787  
r5=1.08905623  
r6=1.08882451  
r7=1.08983544  
a5=112.5827662  
a6=109.69139552  
a7=108.52697728  
d5=49.64766555  
d6=-72.22873273  
d7=170.22268137  
r8=1.08883117  
r9=1.08909883  
r10=1.08977628

a8=109.65908909  
a9=112.56963077  
a10=108.57362342  
d8=169.1991499  
d9=47.377798  
d10=-73.23968745

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C2H7P1\ROSMUS\11-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\PC,1,r2\C,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=1.84852576\r3=1.84869811\r4=1.41360179\ a3=99.17977244\ a4=96.93712075\ d4=98.18077787\r5=1.08905623\r6=1.08882451\r7=1.08983544\ a5=112.5827662\ a6=109.69139552\ a7=108.52697728\ d5=49.64766555\ d6=-72.22873273\ d7=170.22268137\r8=1.08883117\r9=1.08909883\r10=1.08977628\ a8=109.65908909\ a9=112.56963077\ a10=108.57362342\ d8=169.1991499\ d9=47.377798\ d10=-73.23968745\ \Version=IA64L-G09RevA.02\State=1-A\HF=-421.7458737\RMSD=7.254e-09\RMSF=6.258e-05\Dipole=0.3578485,-0.1670525,0.3049791\Quadrupole=-0.2681746,0.1234261,0.1447485,0.7684444,-1.2767202,0.6561119\PG=C01 [X(C2H7P1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C2H7P1\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\PC,1,1.8485257554\C,1,1.8486981063,2,99.17977244\H,1,1.4136017942,2,96.93712075,3,98.18077787,0\H,2,1.0890562253,1,112.5827662,4,49.64766555,0\H,2,1.0888245113,1,109.69139552,4,-72.22873273,0\H,2,1.0898354407,1,108.52697728,4,170.22268137,0\H,3,1.0888311686,1,109.65908909,2,169.1991499,0\H,3,1.0890988311,1,112.56963077,2,47.377798,0\H,3,1.0897762825,1,108.57362342,2,-73.23968745,0\ \Version=IA64L-G09RevA.02\State=1-A\HF=-420.602239\RMSD=6.629e-09\Dipole=0.3824734,-0.186527,0.3259407\Quadrupole=-0.3060125,0.1849556,0.121057,0.8482649,-1.3204402,0.7239587\PG=C01 [X(C2H7P1)]\@\

HF=-421.7458737

Sum of electronic and zero-point Energies= -421.662007  
Sum of electronic and thermal Energies= -421.656767  
Sum of electronic and thermal Enthalpies= -421.655822  
Sum of electronic and thermal Free Energies= -421.689443  
NImag=0

Cl2H1P1

-----  
0,1

P  
Cl,1,r2  
Cl,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=2.05535989  
r3=2.05529174  
r4=1.41243  
a3=101.97876713  
a4=94.78666908  
d4=95.92614217

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Cl2H1P1\ROSMUS\11-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Cl,1,r2\Cl,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=2.05535989\r3=2.05529174\r4=1.41243\ a3=101.97876713\ a4=94.78666908\ d4=95.92614217\Version=IA64L-G09RevA.02\State=1-A\HF=-1262.3853418\RMSD=3.992e-09\RMSF=1.168e-04\Dipole=-0.3357523,-0.2545612,-0.2721222\Quadrupole=0.0929439,0.1435828,-0.2365267,0.7977324,0.7765362,0.6463375\PG=C01 [X(Cl2H1P1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl2H1P1\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\Cl,1,2.055359887\Cl,1,2.0552917389,2,101.97876713\H,1,1.4124299996,2,94.78666908,3,95.92614217,0\Version=IA64L-G09RevA.02\State=1-A\HF=-1260.4273331\RMSD=1.818e-09\Dipole=-0.3732682,-0.2886028,-0.3025198\Quadrupole=-0.005342,0.3992939,-0.3939518,0.9047481,0.9158349,0.7330235\PG=C01 [X(Cl2H1P1)]\@\

HF=-1262.3853418

Sum of electronic and zero-point Energies= -1262.372953  
Sum of electronic and thermal Energies= -1262.369026  
Sum of electronic and thermal Enthalpies= -1262.368082  
Sum of electronic and thermal Free Energies= -1262.400945  
NImag=0

F2H1P1

-----  
0,1  
P  
F,1,r2  
F,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.58835977  
r3=1.58833695  
r4=1.42057606  
a3=98.43867861  
a4=95.38040619  
d4=96.26485487

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\F2H1P1\ROSMUS\11-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\F,1,r2\F,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.58835977\r3=1.58833695\r4=1.42057606\a3=98.43867861\a4=95.38040619\d4=96.26485487\Version=IA64L-G09RevA.02\State=1-A\HF=-541.6884665\RMSD=8.504e-09\RMSF=2.254e-04\Dipole=-0.3835265,-0.2482142,-0.3308741\Quadrupole=-0.292582,0.7428251,-0.4502431,0.6547229,0.5312567,0.5647498\PG=C01 [X(F2H1P1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F2H1P1\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\F,1,1.5883597749\F,1,1.5883369454,2,98.43867861\H,1,1.4205760626,2,95.38040619,3,96.26485487,0\Version=IA64L-G09RevA.02\State=1-A\HF=-540.3669577\RMSD=7.689e-09\Dipole=-0.4301263,-0.2690264,-0.3710733\Quadrupole=-0.3486973,0.8716704,-0.522973,0.7496344,0.5872386,0.64661\PG=C01 [X(F2H1P1)]\@

HF=-541.6884665

Sum of electronic and zero-point Energies=	-541.673479
Sum of electronic and thermal Energies=	-541.670098
Sum of electronic and thermal Enthalpies=	-541.669154
Sum of electronic and thermal Free Energies=	-541.699186
NImag=0	

Ge2H7P1

-----

0,1  
P  
Ge,1,r2  
Ge,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0



r2=2.33070442  
r3=2.33050326  
r4=1.41317806  
a3=95.8867548  
a4=93.84070531  
d4=265.67464366  
r5=1.54144726  
r6=1.5439034  
r7=1.54294496  
a5=108.89098624  
a6=112.06072316  
a7=107.49395318  
d5=76.8504384  
d6=-44.62050447  
d7=195.44864049  
r8=1.54429545  
r9=1.54152939  
r10=1.54252237  
a8=112.25837025  
a9=108.61485519  
a10=107.49497695  
d8=315.19767942  
d9=193.87487059  
d10=75.35810522

--- Geometry Optimization ---

```
1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Ge2H7P1\ROSMUS\12-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\P\Ge,1,r2\Ge,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,
d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=2
.33070442\r3=2.33050326\r4=1.41317806\a3=95.8867548\a4=93.84070531\d4=265.674
64366\r5=1.54144726\r6=1.5439034\r7=1.54294496\a5=108.89098624\a6=112.0607231
6\a7=107.49395318\d5=76.8504384\d6=-
44.62050447\d7=195.44864049\r8=1.54429545\r9=1.54152939\r10=1.54252237\a8=112
.25837025\a9=108.61485519\a10=107.49497695\d8=315.19767942\d9=193.87487059\d
10=75.35810522\Version=IA64L-G09RevA.02\State=1-A\HF=-
4499.4856627\RMSD=8.139e-09\RMSF=3.068e-
05\Dipole=0.14245,0.1725883,0.1296636\Quadrupole=-0.3614106,0.5158847,-
0.154474,-0.7359302,-1.1054475,-0.6595528\PG=C01 [X(Ge2H7P1)]\@
```

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge2H7P1\ROSMUS\18-Dec-2012\0\#p hf cc-
pvqz scf=verytight guess=read geom=allcheck
pop=savenbos\title\0,1\P\Ge,1,2.3307044179\Ge,1,2.3305032613,2,95.8867548\H,1,1.4
131780589,2,93.84070531,3,265.67464366,0\H,2,1.5414472562,1,108.89098624,4,76.85
04384,0\H,2,1.5439034024,1,112.06072316,4,-
```

44.62050447,0\H,2,1.542944963,1,107.49395318,4,195.44864049,0\H,3,1.5442954455,1  
,112.25837025,2,315.19767942,0\H,3,1.5415293908,1,108.61485519,2,193.87487059,0\  
H,3,1.5425223652,1,107.49497695,2,75.35810522,0\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-4495.6541214\RMSD=3.251e-  
09\Dipole=0.1583812,0.2082306,0.1450311\Quadrupole=-0.4480738,0.6979281,-  
0.2498542,-0.808912,-1.0748201,-0.7248172\PG=C01 [X(Ge2H7P1)]\@

HF=-4499.4856627

Sum of electronic and zero-point Energies= -4499.429156  
Sum of electronic and thermal Energies= -4499.421641  
Sum of electronic and thermal Enthalpies= -4499.420696  
Sum of electronic and thermal Free Energies= -4499.464058  
NImag=0

H3O2P1

-----  
0,1  
P  
O,1,r2  
O,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.63972778  
r3=1.63963222  
r4=1.40734273  
r5=0.95886818  
r6=0.95886925  
a3=103.44082339  
a4=93.93254839  
a5=111.75668656  
a6=111.77764657  
d4=94.95730976  
d5=203.23963646  
d6=252.04683189

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O2P1\ROSMUS\11-Dec-  
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\title\\0,1\O,1,r2\O,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6  
,0\r2=1.63972778\r3=1.63963222\r4=1.40734273\r5=0.95886818\r6=0.95886925\a3=10  
3.44082339\a4=93.93254839\a5=111.75668656\a6=111.77764657\d4=94.95730976\d5=  
203.23963646\d6=252.04683189\\Version=IA64L-G09RevA.02\State=1-A\HF=-

493.6334154\RMSD=6.790e-09\RMSF=3.509e-05\Dipole=-0.1200418,0.7967234,-  
0.0928483\Quadrupole=-1.0810038,1.3742004,-0.2931966,1.7516885,-  
1.6832672,1.3825362\PG=C01 [X(H3O2P1)]\ \@  
--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O2P1\ROSMUS\18-Dec-2012\0\#p hf cc-  
pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\O,1,1.6397277773\O,1,1.6396322236,2,103.44082339\H,1,1.4  
073427331,2,93.93254839,3,94.95730976,0\H,2,0.9588681775,1,111.75668656,4,203.23  
963646,0\H,3,0.9588692526,1,111.77764657,2,252.04683189,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-492.3408746\RMSD=2.882e-09\Dipole=-  
0.1500903,0.8235117,-0.1164567\Quadrupole=-1.1018435,1.4285993,-  
0.3267557,1.8606,-1.6574539,1.4682995\PG=C01 [X(H3O2P1)]\ \@

HF=-493.6334154

Sum of electronic and zero-point Energies=	-493.594121
Sum of electronic and thermal Energies=	-493.589971
Sum of electronic and thermal Enthalpies=	-493.589027
Sum of electronic and thermal Free Energies=	-493.620180
NImag=0	

H3P1Se2

-----  
0,1  
P  
Se,1,r2  
Se,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=2.26917263  
r3=2.26925478  
r4=1.40655021  
r5=1.46596153  
r6=1.46593392  
a3=106.60987212  
a4=92.91512964  
a5=92.12503384  
a6=92.11347907  
d4=93.92926405  
d5=204.81511908  
d6=249.062092

--- Geometry Optimization ---

```

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3P1Se2\ROSMUS\11-Dec-
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\P\Se,1,r2\Se,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d
6,0\r2=2.26917263\r3=2.26925478\r4=1.40655021\r5=1.46596153\r6=1.46593392\a3=1
06.60987212\a4=92.91512964\a5=92.12503384\a6=92.11347907\d4=93.92926405\d5=2
04.81511908\d6=249.062092\Version=IA64L-G09RevA.02\State=1-A\HF=-
5146.2790232\RMSD=8.919e-09\RMSF=1.225e-04\Dipole=-0.1787826,0.2329151,-
0.1332181\Quadrupole=-1.4451501,2.5320623,-1.0869122,-0.0194988,-0.5959552,-
0.0151346\PG=C01 [X(H3P1Se2)]\@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3P1Se2\ROSMUS\18-Dec-2012\0\#p hf cc-
pvqz scf=verytight guess=read geom=allcheck
pop=savenbos\title\0,1\P\Se,1,2.2691726289\Se,1,2.2692547791,2,106.60987212\H,1,1
.4065502071,2,92.91512964,3,93.92926405,0\H,2,1.4659615259,1,92.12503384,4,204.8
1511908,0\H,3,1.4659339172,1,92.11347907,2,249.062092,0\Version=IA64L-
G09RevA.02\State=1-A\HF=-5142.3106658\RMSD=3.908e-09\Dipole=-
0.185297,0.2312328,-0.1381025\Quadrupole=-1.5477967,2.7437435,-
1.1959468,0.1338018,-0.5850188,0.099158\PG=C01 [X(H3P1Se2)]\@

```

HF=-5146.2790232

```

Sum of electronic and zero-point Energies=      -5146.251319
Sum of electronic and thermal Energies=         -5146.246049
Sum of electronic and thermal Enthalpies=       -5146.245105
Sum of electronic and thermal Free Energies=    -5146.282329
NImag=0

```

H7P1Si2

```

-----
0,1
P
Si,1,r2
Si,1,r3,2,a3
H,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,2,r6,1,a6,4,d6,0
H,2,r7,1,a7,4,d7,0
H,3,r8,1,a8,2,d8,0
H,3,r9,1,a9,2,d9,0
H,3,r10,1,a10,2,d10,0

```

```

r2=2.25097421
r3=2.25098388
r4=1.41399705
a3=95.49115671

```

a4=94.41521841  
d4=265.13542119  
r5=1.47617271  
r6=1.47820038  
r7=1.47663359  
a5=108.92927246  
a6=113.03758053  
a7=107.3464889  
d5=73.43470773  
d6=-48.09551965  
d7=191.76240136  
r8=1.47817314  
r9=1.47620038  
r10=1.47665297  
a8=113.02729362  
a9=108.92689693  
a10=107.36124775  
d8=312.95564726  
d9=191.43884736  
d10=73.10983988

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H7P1Si2\ROSMUS\12-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Si,1,r2\Si,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\|r2=2.25097421|r3=2.25098388|r4=1.41399705|a3=95.49115671|a4=94.41521841|d4=265.13542119|r5=1.47617271|r6=1.47820038|r7=1.47663359|a5=108.92927246|a6=113.03758053|a7=107.3464889|d5=73.43470773|d6=-48.09551965|d7=191.76240136|r8=1.47817314|r9=1.47620038|r10=1.47665297|a8=113.02729362|a9=108.92689693|a10=107.36124775|d8=312.95564726|d9=191.43884736|d10=73.10983988\|Version=IA64L-G09RevA.02\State=1-A\HF=-924.4993845\RMSD=3.205e-09\RMSF=2.264e-05\Dipole=0.1244111,0.1829777,0.1130885\Quadrupole=-0.3394142,0.5149598,-0.1755456,-0.6959351,-0.8514382,-0.6316603\PG=C01 [X(H7P1Si2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H7P1Si2\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\Si,1,2.2509742082\Si,1,2.2509838812,2,95.49115671\H,1,1.4139970539,2,94.41521841,3,265.13542119,0\H,2,1.4761727149,1,108.92927246,4,73.43470773,0\H,2,1.4782003822,1,113.03758053,4,-48.09551965,0\H,2,1.4766335917,1,107.3464889,4,191.76240136,0\H,3,1.4781731414,1,113.02729362,2,312.95564726,0\H,3,1.4762003803,1,108.92689693,2,191.43884736,0\H,3,1.4766529725,1,107.36124775,2,73.10983988,0\|Version=IA64L-G09RevA.02\State=1-A\HF=-922.7373603\RMSD=6.274e-

09\Dipole=0.1480183,0.2189985,0.1345278\Quadrupole=-0.4202175,0.6687383,-  
0.2485208,-0.7596679,-0.8925761,-0.6895754\PG=C01 [X(H7P1Si2)]\@

HF=-924.4993845

Sum of electronic and zero-point Energies= -924.439219  
Sum of electronic and thermal Energies= -924.432318  
Sum of electronic and thermal Enthalpies= -924.431374  
Sum of electronic and thermal Free Energies= -924.470548  
NImag=0

H3P1S2

-----  
0,1  
P  
S,1,r2  
S,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=2.11465038  
r3=2.1148034  
r4=1.4057911  
r5=1.3394092  
r6=1.3393807  
a3=107.13305937  
a4=97.5801963  
a5=99.37862637  
a6=99.36108892  
d4=259.7062433  
d5=319.33828471  
d6=300.36240558

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3P1S2\ROSMUS\11-Dec-  
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\S,1,r2\S,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,  
0\r2=2.11465038\r3=2.1148034\r4=1.4057911\r5=1.3394092\r6=1.3393807\a3=107.133  
05937\a4=97.5801963\a5=99.37862637\a6=99.36108892\d4=259.7062433\d5=319.3382  
8471\d6=300.36240558\Version=IA64L-G09RevA.02\State=1-A\HF=-  
1139.5447542\RMSD=9.834e-09\RMSF=6.483e-  
05\Dipole=0.1150389,0.7216479,0.0856711\Quadrupole=-0.4711761,1.6625485,-  
1.1913724,1.2167476,1.1747342,0.8974401\PG=C01 [X(H3P1S2)]\@  
--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3P1S2\ROSMUS\18-Dec-2012\0\#p hf cc-  
pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\S,1,2.1146503776\S,1,2.1148034027,2,107.13305937\H,1,1.4  
05791098,2,97.5801963,3,259.7062433,0\H,2,1.3394091997,1,99.37862637,4,319.33828  
471,0\H,3,1.3393806967,1,99.36108892,2,300.36240558,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-1137.632898\RMSD=6.672e-  
09\Dipole=0.1263918,0.8086342,0.094075\Quadrupole=-0.5253317,1.8862928,-  
1.3609611,1.1546461,1.3623256,0.8516889\PG=C01 [X(H3P1S2)]\@

HF=-1139.5447542

Sum of electronic and zero-point Energies= -1139.515300  
Sum of electronic and thermal Energies= -1139.510226  
Sum of electronic and thermal Enthalpies= -1139.509282  
Sum of electronic and thermal Free Energies= -1139.544005  
NImag=0

Br3P1

-----  
0,1  
P  
Br,1,r2  
Br,1,r3,2,a3  
Br,1,r4,2,a4,3,d4,0  
  
r2=2.22472519  
r3=2.22564659  
r4=2.22564668  
a3=101.0214886  
a4=101.02142373  
d4=103.58695467

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Br3P1\ROSMUS\13-Dec-  
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Br,1,r2\Br,1,r3,2,a3\Br,1,r4,2,a4,3,d4,0\r2=2.22472519\r3=2.22564659\  
r4=2.22564668\a3=101.0214886\a4=101.02142373\d4=103.58695467\Version=IA64L-  
G09RevA.02\State=1-A\HF=-8063.9388076\RMSD=5.882e-09\RMSF=7.043e-  
05\Dipole=-0.1081589,0.1374127,-0.0876059\Quadrupole=0.0014096,0.0001286,-  
0.0015382,0.0025176,-0.0048981,0.0062729\PG=C01 [X(Br3P1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br3P1\ROSMUS\18-Dec-2012\0\#p hf cc-  
pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\Br,1,2.2247251914\Br,1,2.2256465851,2,101.0214886\Br,1,2.  
2256466799,2,101.02142373,3,103.58695467,0\Version=IA64L-G09RevA.02\State=1-

A\HF=-8058.2194782\RMSD=3.431e-09\Dipole=-0.1084488,0.1377822,-  
0.0867027\Quadrupole=-0.0046036,0.0079071,-0.0033035,-0.025883,0.012119,-  
0.0154005\PG=C01 [X(Br3P1)]\@

HF=-8063.9388076

Sum of electronic and zero-point Energies= -8063.935127  
Sum of electronic and thermal Energies= -8063.929356  
Sum of electronic and thermal Enthalpies= -8063.928412  
Sum of electronic and thermal Free Energies= -8063.968814  
NImag=0

C3H9P1

-----  
0,1  
P  
C,1,r2  
C,1,r3,2,a3  
C,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0  
H,4,r11,1,a11,3,d11,0  
H,4,r12,1,a12,3,d12,0  
H,4,r13,1,a13,3,d13,0

r2=1.84389139  
r3=1.84372127  
r4=1.84400701  
a3=98.90367774  
a4=98.85469235  
d4=100.24081677  
r5=1.09178908  
r6=1.08974254  
r7=1.08962851  
a5=111.71294248  
a6=109.43385772  
a7=109.54116811  
d5=51.03882671  
d6=-69.82071309  
d7=172.00024888  
r8=1.08967434



r9=1.0918747  
r10=1.08982214  
a8=109.506488  
a9=111.67656  
a10=109.50482837  
d8=172.13256499  
d9=51.23362779  
d10=-69.6380014  
r11=1.09185538  
r12=1.08971757  
r13=1.08957602  
a11=111.69878374  
a12=109.35560498  
a13=109.67480918  
d11=51.79544518  
d12=-68.90063991  
d13=172.87217876

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C3H9P1\ROSMUS\13-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\PC,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.84389139\r3=1.84372127\r4=1.84400701\a3=98.90367774\a4=98.85469235\d4=100.24081677\r5=1.09178908\r6=1.08974254\r7=1.08962851\a5=111.71294248\a6=109.43385772\a7=109.54116811\d5=51.03882671\d6=-69.82071309\d7=172.00024888\r8=1.08967434\r9=1.0918747\r10=1.08982214\a8=109.506488\a9=111.67656\a10=109.50482837\d8=172.13256499\d9=51.23362779\d10=-69.6380014\r11=1.09185538\r12=1.08971757\r13=1.08957602\a11=111.69878374\a12=109.35560498\a13=109.67480918\d11=51.79544518\d12=-68.90063991\d13=172.87217876\Version=IA64L-G09RevA.02\State=1-A\HF=-461.0617729\RMSD=5.304e-09\RMSF=9.355e-05\Dipole=0.2708346,-0.3231544,0.2314145\Quadrupole=0.0555883,-0.4012351,0.3456467,1.2635397,-0.9063177,1.082893\PG=C01 [X(C3H9P1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C3H9P1\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\PC,1,1.8438913863\C,1,1.8437212652,2,98.90367774\C,1,1.8440070062,2,98.85469235,3,100.24081677,0\H,2,1.0917890844,1,111.71294248,4,51.03882671,0\H,2,1.0897425414,1,109.43385772,4,-69.82071309,0\H,2,1.0896285128,1,109.54116811,4,172.00024888,0\H,3,1.089674339,1,109.506488,2,172.13256499,0\H,3,1.0918747018,1,111.67656,2,51.23362779,0\H,3,1.0898221361,1,109.50482837,2,-69.6380014,0\H,4,1.0918553826,1,111.69878374,3,51.79544518,0\H,4,1.0897175736,1,109.35560498,3,-

68.90063991,0\H,4,1.0895760181,1,109.67480918,3,172.87217876,0\Version=IA64L-G09RevA.02\State=1-A\HF=-459.659319\RMSD=2.868e-09\Dipole=0.299966,-0.3582098,0.2567933\Quadrupole=0.0585964,-0.4182906,0.3596942,1.3186531,-0.9449331,1.1294378\PG=C01 [X(C3H9P1)]\@

HF=-461.0617729

Sum of electronic and zero-point Energies= -460.949105  
Sum of electronic and thermal Energies= -460.942397  
Sum of electronic and thermal Enthalpies= -460.941453  
Sum of electronic and thermal Free Energies= -460.978451  
NImag=0

Cl3P1

-----  
0,1  
P  
Cl,1,r2  
Cl,1,r3,2,a3  
Cl,1,r4,2,a4,3,d4,0

r2=2.04697263  
r3=2.04786691  
r4=2.04786691  
a3=100.01732369  
a4=100.01731577  
d4=102.16896563

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Cl3P1\ROSMUS\13-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Cl,1,r2\Cl,1,r3,2,a3\Cl,1,r4,2,a4,3,d4,0\r2=2.04697263\r3=2.04786691\r4=2.04786691\a3=100.01732369\a4=100.01731577\d4=102.16896563\Version=IA64L-G09RevA.02\State=1-A\HF=-1722.0234207\RMSD=6.223e-09\RMSF=1.872e-04\Dipole=-0.128983,0.1597613,-0.1064534\Quadrupole=-0.0037261,0.0169493,-0.0132232,-0.0479201,0.0298524,-0.0369771\PG=C01 [X(Cl3P1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl3P1\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\Cl,1,2.0469726347\Cl,1,2.0478669111,2,100.01732369\Cl,1,2.0478669098,2,100.01731577,3,102.16896563,0\Version=IA64L-G09RevA.02\State=1-A\HF=-1719.396966\RMSD=4.917e-09\Dipole=-0.143778,0.1780873,-0.118422\Quadrupole=-0.0097341,0.0429898,-0.0332557,-0.1222495,0.0808165,-0.1001017\PG=C01 [X(Cl3P1)]\@

HF=-1722.0234207

Sum of electronic and zero-point Energies= -1722.018456  
Sum of electronic and thermal Energies= -1722.013348  
Sum of electronic and thermal Enthalpies= -1722.012403  
Sum of electronic and thermal Free Energies= -1722.048774  
NImag=0

F3P1

-----  
0,1  
P  
F,1,r2  
F,1,r3,2,a3  
F,1,r4,2,a4,3,d4,0

r2=1.57036472  
r3=1.57077391  
r4=1.57077393  
a3=97.16125731  
a4=97.1612521  
d4=98.12257538

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\F3P1\ROSMUS\13-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\#P\F,1,r2\F,1,r3,2,a3\F,1,r4,2,a4,3,d4,0\r2=1.57036472\r3=1.57077391\r4=1.57077393\a3=97.16125731\a4=97.1612521\d4=98.12257538\Version=IA64L-G09RevA.02\State=1-A\HF=-641.0021554\RMSD=5.368e-09\RMSF=1.330e-04\Dipole=-0.2597799,0.2994893,-0.2263438\Quadrupole=-0.0066093,0.0542029,-0.0475936,-0.2130451,0.1605041,-0.1850385\PG=C01 [X(F3P1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F3P1\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz  
scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\#P\F,1,1.5703647219\F,1,1.5707739087,2,97.16125731\F,1,1.5707739254,2,97.1612521,3,98.12257538,0\Version=IA64L-G09RevA.02\State=1-A\HF=-639.3339033\RMSD=3.291e-09\Dipole=-0.2852224,0.3288207,-0.2497575\Quadrupole=-0.0065937,0.050333,-0.0437392,-0.1994308,0.1534924,-0.1769546\PG=C01 [X(F3P1)]\@

HF=-641.0021554

Sum of electronic and zero-point Energies= -640.993460  
Sum of electronic and thermal Energies= -640.989476  
Sum of electronic and thermal Enthalpies= -640.988532

Sum of electronic and thermal Free Energies= -641.020565  
NImag=0

Ge3H9P1

-----  
0,1  
P  
Ge,1,r2  
Ge,1,r3,2,a3  
Ge,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0  
H,4,r11,1,a11,3,d11,0  
H,4,r12,1,a12,3,d12,0  
H,4,r13,1,a13,3,d13,0

r2=2.27977107  
r3=2.28014675  
r4=2.28037481  
a3=120.04765679  
a4=119.90504793  
d4=179.94383007  
r5=1.54190284  
r6=1.5418422  
r7=1.54186663  
a5=111.24237718  
a6=104.70463142  
a7=111.21448195  
d5=118.97052579  
d6=-0.18732923  
d7=240.66569412  
r8=1.54187459  
r9=1.54188607  
r10=1.54187559  
a8=111.10796444  
a9=111.11750689  
a10=104.75473495  
d8=240.67260981  
d9=119.0722721  
d10=-0.12278576  
r11=1.54197899

r12=1.54160724  
r13=1.54210261  
a11=111.04477312  
a12=104.86189631  
a13=111.17584558  
d11=119.50310249  
d12=0.38521661  
d13=241.21660697

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Ge3H9P1\ROSMUS\13-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\Ge,1,r2\Ge,1,r3,2,a3\Ge,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=2.27977107\r3=2.28014675\r4=2.28037481\a3=120.04765679\a4=119.90504793\d4=179.94383007\r5=1.54190284\r6=1.5418422\r7=1.54186663\a5=111.24237718\a6=104.70463142\a7=111.21448195\d5=118.97052579\d6=-0.18732923\d7=240.66569412\r8=1.54187459\r9=1.54188607\r10=1.54187559\a8=111.10796444\a9=111.11750689\a10=104.75473495\d8=240.67260981\d9=119.0722721\d10=-0.12278576\r11=1.54197899\r12=1.54160724\r13=1.54210261\a11=111.04477312\a12=104.86189631\a13=111.17584558\d11=119.50310249\d12=0.38521661\d13=241.21660697\Version=IA64L-G09RevA.02\State=1-A\HF=-6577.6446089\RMSD=9.819e-09\RMSF=1.666e-04\Dipole=0.0010941,-0.0000689,-0.0029726\Quadrupole=1.3114589,-2.5947964,1.2833374,0.0029665,0.0000019,0.0015502\PG=C01 [X(Ge3H9P1)]\@\nbo  
--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge3H9P1\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\0,1\P\Ge,1,2.2797710692\Ge,1,2.2801467538,2,120.04765679\Ge,1,2.280374809,2,119.90504793,3,179.94383007,0\H,2,1.5419028407,1,111.24237718,4,118.97052579,0\H,2,1.5418421953,1,104.70463142,4,-0.18732923,0\H,2,1.5418666279,1,111.21448195,4,240.66569412,0\H,3,1.5418745896,1,111.10796444,2,240.67260981,0\H,3,1.5418860682,1,111.11750689,2,119.0722721,0\H,3,1.5418755886,1,104.75473495,2,-0.12278576,0\H,4,1.5419789939,1,111.04477312,3,119.50310249,0\H,4,1.5416072414,1,104.86189631,3,0.38521661,0\H,4,1.5421026131,1,111.17584558,3,241.21660697,0\Version=IA64L-G09RevA.02\State=1-A\HF=-6572.2151333\RMSD=3.531e-09\Dipole=0.002212,-0.0000021,-0.0026936\Quadrupole=1.1571319,-2.2879098,1.1307779,0.0023814,-0.0013246,0.0011809\PG=C01 [X(Ge3H9P1)]\@\nbo

HF=-6577.6446089

Sum of electronic and zero-point Energies= -6577.572379  
Sum of electronic and thermal Energies= -6577.563486

Sum of electronic and thermal Enthalpies= -6577.562542  
Sum of electronic and thermal Free Energies= -6577.609941  
NImag=2

### H3O3P1

-----  
0,1  
P  
O,1,r2  
O,1,r3,2,a3  
O,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0  
H,4,r7,1,a7,3,d7,0

r2=1.62439072  
r3=1.62391082  
r4=1.62415712  
r5=0.95994939  
r6=0.96004198  
r7=0.96000459  
a3=97.58040271  
a4=97.65172859  
a5=112.42813757  
a6=112.44224398  
a7=112.45463026  
d4=98.77260133  
d5=197.52635852  
d6=196.78681317  
d7=196.54793421

### --- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O3P1\ROSMUS\13-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\O,1,r2\O,1,r3,2,a3\O,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\H,4,r7,1,a7,3,d7,0\r2=1.62439072\r3=1.62391082\r4=1.62415712\r5=0.95994939\r6=0.96004198\r7=0.96000459\a3=97.58040271\a4=97.65172859\a5=112.42813757\a6=112.44224398\a7=112.45463026\d4=98.77260133\d5=197.52635852\d6=196.78681317\d7=196.54793421\Version=IA64L-G09RevA.02\State=1-A\HF=-568.9079684\RMSD=3.627e-09\RMSF=1.300e-04\Dipole=-0.547057,0.6290876,-0.4711616\Quadrupole=0.1079162,-0.6827041,0.5747879,2.4622626,-1.8993643,2.1593817\PG=C01 [X(H3O3P1)]\@

### --- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O3P1\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck

pop=savenbos\\title\\0,1\P\O,1,1.6243907154\O,1,1.6239108171,2,97.58040271\O,1,1.6241571189,2,97.65172859,3,98.77260133,0\H,2,0.9599493911,1,112.42813757,4,197.52635852,0\H,3,0.9600419836,1,112.44224398,2,196.78681317,0\H,4,0.9600045909,1,112.45463026,3,196.54793421,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-567.2841703\RMSD=9.081e-09\Dipole=-0.5863009,0.6744698,-0.5062576\Quadrupole=0.1084487,-0.6974372,0.5889885,2.5140423,-1.9378885,2.2038498\PG=C01 [X(H3O3P1)]\\@

HF=-568.9079684

Sum of electronic and zero-point Energies= -568.864004  
Sum of electronic and thermal Energies= -568.858288  
Sum of electronic and thermal Enthalpies= -568.857344  
Sum of electronic and thermal Free Energies= -568.892497  
NImag=0

H3P1Se3

-----  
0,1  
P  
X,1,1.  
Se,1,rS,2,aS  
Se,1,rS,2,aS,3,dS,0  
Se,1,rS,2,aS,3,-dS,0  
H,3,rH,1,aH,2,dH,0  
H,4,rH,1,aH,2,dH,0  
H,5,rH,1,aH,2,dH,0

rS=2.2615762  
rH=1.47090858  
aS=114.06278331  
aH=96.77947541  
dS=120.  
dH=180.

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3P1Se3\ROSMUS\13-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\title\\0,1\P\X,1,1.\Se,1,rS,2,aS\Se,1,rS,2,aS,3,dS,0\Se,1,rS,2,aS,3,-dS,0\H,3,rH,1,aH,2,dH,0\H,4,rH,1,aH,2,dH,0\H,5,rH,1,aH,2,dH,0\rS=2.2615762\rH=1.47090858\aS=114.06278331\aH=96.77947541\dS=120.\dH=180.\\Version=IA64L-G09RevA.02\State=1-A1\HF=-7547.8523219\RMSD=1.956e-09\RMSF=6.911e-06\Dipole=0.,0.,-0.6065278\Quadrupole=-2.0733946,-2.0733946,4.1467892,0.,0.,0.\PG=C03V [C3(P1),3SGV(H1Se1)]\\@

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3P1Se3\ROSMUS\18-Dec-2012\0\#p hf cc-
pvqz scf=verytight guess=read geom=allcheck
pop=savenbos\title\0,1\X,1,1.\Se,1,2.2615761992,2,114.06278331\Se,1,2.261576199
2,2,114.06278331,3,120.,0\Se,1,2.2615761992,2,114.06278331,3,-
120.,0\H,3,1.4709085762,1,96.77947541,2,180.,0\H,4,1.4709085762,1,96.77947541,2,18
0.,0\H,5,1.4709085762,1,96.77947541,2,180.,0\Version=IA64L-G09RevA.02\State=1-
A1\HF=-7542.2132655\RMSD=5.074e-09\Dipole=0.,0.,-0.6890696\Quadrupole=-
2.1579467,-2.1579467,4.3158934,0.,0.,0.\PG=C03V [C3(P1),3SGV(H1Se1)]\@
```

HF=-7547.8523219

```
Sum of electronic and zero-point Energies=      -7547.826460
Sum of electronic and thermal Energies=         -7547.818088
Sum of electronic and thermal Enthalpies=       -7547.817144
Sum of electronic and thermal Free Energies=    -7547.862352
NImag=0
```

Br2H1O1(1+)

```
-----
1,1
O
Br,1,r2
Br,1,r3,2,a3
H,1,r4,2,a4,3,d4,0

r2=1.87535478
r3=1.87583016
r4=0.97828625
a3=118.34593093
a4=108.88986669
d4=124.89546583
```

--- Geometry Optimization ---

```
1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Br2H1O1(1+)\ROSMUS\11-
Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\1,1\O\Br,1,r2\Br,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.87535478\r3=1.87583016\r
4=0.97828625\a3=118.34593093\a4=108.88986669\d4=124.89546583\Version=IA64L-
G09RevA.02\State=1-A\HF=-5223.7185642\RMSD=4.386e-09\RMSF=2.711e-
04\Dipole=-0.466899,-0.4940258,-0.2791788\Quadrupole=0.4727653,-
4.8864696,4.4137042,1.7991117,-3.6528395,1.074479\PG=C01 [X(Br2H1O1)]\@
```

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br2H1O1(1+)\ROSMUS\18-Dec-2012\0\#p
hf cc-pvqz scf=verytight guess=read geom=allcheck
pop=savenbos\title\1,1\O\Br,1,1.8753547781\Br,1,1.8758301586,2,118.34593093\H,1,0
```



.9782862477,2,108.88986669,3,124.89546583,0\\Version=IA64L-G09RevA.02\\State=1-A\\HF=-5219.9802527\\RMSD=3.597e-09\\Dipole=-0.4244489,-0.5139816,-0.2542874\\Quadrupole=0.4249687,-4.9073032,4.4823345,1.7873739,-3.7608142,1.067555\\PG=C01 [X(Br2H1O1)]\\@

HF=-5223.7185642

Sum of electronic and zero-point Energies= -5223.702835  
Sum of electronic and thermal Energies= -5223.698903  
Sum of electronic and thermal Enthalpies= -5223.697959  
Sum of electronic and thermal Free Energies= -5223.731971  
NImag=0

C2H7O1(1+)

-----  
1,1  
O  
C,1,r2  
C,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0

r2=1.47517967  
r3=1.47518226  
r4=0.97058089  
a3=116.39112958  
a4=112.41117957  
d4=131.69277637  
r5=1.08675636  
r6=1.08463883  
r7=1.08470708  
a5=108.66314236  
a6=106.1335635  
a7=105.37411516  
d5=71.75223612  
d6=-49.56676976  
d7=192.30784033  
r8=1.08463656  
r9=1.08676198  
r10=1.08469813

a8=106.13428882  
a9=108.66118148  
a10=105.37430916  
d8=181.03589732  
d9=59.72205925  
d10=-60.83993366

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C2H7O1(1+)\ROSMUS\11-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\C,1,r2\C,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=1.47517967\r3=1.47518226\r4=0.97058089\ a3=116.39112958\ a4=112.41117957\d4=131.69277637\r5=1.08675636\r6=1.08463883\r7=1.08470708\ a5=108.66314236\ a6=106.1335635\ a7=105.37411516\d5=71.75223612\d6=-49.56676976\d7=192.30784033\r8=1.08463656\r9=1.08676198\r10=1.08469813\ a8=106.13428882\ a9=108.66118148\ a10=105.37430916\d8=181.03589732\d9=59.72205925\d10=-60.83993366\Version=IA64L-G09RevA.02\State=1-A\HF=-155.3164743\RMSD=9.573e-09\RMSF=6.054e-05\Dipole=-0.1722836,-0.414056,-0.1068516\Quadrupole=0.3008882,-2.1340722,1.8331839,1.3381812,-1.5437902,0.8301563\PG=C01 [X(C2H7O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C2H7O1(1+)\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\C,1,1.4751796725\C,1,1.4751822623,2,116.39112958\H,1,0.9705808908,2,112.41117957,3,131.69277637,0\H,2,1.0867563599,1,108.66314236,4,71.75223612,0\H,2,1.0846388302,1,106.1335635,4,-49.56676976,0\H,2,1.0847070772,1,105.37411516,4,192.30784033,0\H,3,1.0846365602,1,106.13428882,2,181.03589732,0\H,3,1.0867619831,1,108.66118148,2,59.72205925,0\H,3,1.084698128,1,105.37430916,2,-60.83993366,0\Version=IA64L-G09RevA.02\State=1-A\HF=-154.4606023\RMSD=7.230e-09\Dipole=-0.1532881,-0.4262316,-0.0950776\Quadrupole=0.293977,-2.1024279,1.8084509,1.3406494,-1.5258847,0.8316184\PG=C01 [X(C2H7O1)]\@

HF=-155.3164743

Sum of electronic and zero-point Energies=	-155.222704
Sum of electronic and thermal Energies=	-155.217980
Sum of electronic and thermal Enthalpies=	-155.217035
Sum of electronic and thermal Free Energies=	-155.248694
NImag=0	

Cl2H1O1(1+)

-----

1,1

O  
Cl,1,r2  
Cl,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.71644645  
r3=1.71700856  
r4=0.98512818  
a3=116.01873821  
a4=108.43495479  
d4=122.10072446

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Cl2H1O1(1+)\ROSMUS\11-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Cl,1,r2\Cl,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.71644645\r3=1.71700856\r4=0.98512818\ a3=116.01873821\ a4=108.43495479\ d4=122.10072446\Version=IA64L-G09RevA.02\State=1-A\HF=-995.7291139\RMSD=8.216e-09\RMSF=2.009e-04\Dipole=-0.4762846,-0.5495531,-0.2981451\Quadrupole=0.5931436,-3.4101928,2.8170492,1.7171102,-2.2761523,1.0742665\PG=C01 [X(Cl2H1O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl2H1O1(1+)\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Cl,1,1.7164464497\Cl,1,1.7170085582,2,116.01873821\H,1,0.9851281772,2,108.43495479,3,122.10072446,0\Version=IA64L-G09RevA.02\State=1-A\HF=-994.0421087\RMSD=8.901e-09\Dipole=-0.445776,-0.5722378,-0.279566\Quadrupole=0.5660107,-3.4196567,2.853646,1.7055895,-2.3415201,1.0671736\PG=C01 [X(Cl2H1O1)]\@

HF=-995.7291139

Sum of electronic and zero-point Energies=	-995.712501
Sum of electronic and thermal Energies=	-995.708862
Sum of electronic and thermal Enthalpies=	-995.707918
Sum of electronic and thermal Free Energies=	-995.739296
NImag=0	

F2H1O1(1+)

-----  
1,1  
O  
F,1,r2  
F,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.35655109  
r3=1.35654062  
r4=1.01164023  
a3=106.25794725  
a4=104.04872275  
d4=109.4280864

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\F2H1O1(1+)\ROSMUS\11-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\F,1,r2\F,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.35655109\r3=1.35654062\r4=1.01164023\a3=106.25794725\a4=104.04872275\d4=109.4280864\Version=IA64L-G09RevA.02\State=1-A\HF=-274.8357648\RMSD=4.342e-09\RMSF=6.096e-05\Dipole=-0.7068803,-0.7916617,-0.5305883\Quadrupole=0.1832573,-0.3070337,0.1237764,1.4216473,0.1060234,1.0676509\PG=C01 [X(F2H1O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F2H1O1(1+)\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\F,1,1.3565510935\F,1,1.3565406198,2,106.25794725\H,1,1.0116402334,2,104.04872275,3,109.4280864,0\Version=IA64L-G09RevA.02\State=1-A\HF=-273.7692876\RMSD=3.014e-09\Dipole=-0.7023722,-0.8142869,-0.5271747\Quadrupole=0.1359221,-0.2026566,0.0667344,1.4317064,0.1228538,1.0752455\PG=C01 [X(F2H1O1)]\@

HF=-274.8357648

Sum of electronic and zero-point Energies=	-274.816540
Sum of electronic and thermal Energies=	-274.813402
Sum of electronic and thermal Enthalpies=	-274.812458
Sum of electronic and thermal Free Energies=	-274.841129
NImag=0	

Ge2H7O1(1+)

-----  
1,1  
O  
Ge,1,r2  
Ge,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0

r2=1.92586795  
r3=1.92585961  
r4=0.96476704  
a3=130.69072378  
a4=114.63855286  
d4=180.06754491  
r5=1.5258795  
r6=1.52587489  
r7=1.52596923  
a5=102.15226041  
a6=102.14106407  
a7=99.04340637  
d5=60.49609499  
d6=-60.18983276  
d7=180.15118298  
r8=1.5258708  
r9=1.52588043  
r10=1.52596878  
a8=102.13676285  
a9=102.15822858  
a10=99.04042146  
d8=240.15250067  
d9=119.46472118  
d10=-0.18843236

--- Geometry Optimization ---

```
1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Ge2H7O1(1+)\ROSMUS\11-  
Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Ge,1,r2\Ge,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,  
d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\r2=1  
.92586795\r3=1.92585961\r4=0.96476704\a3=130.69072378\a4=114.63855286\d4=180.  
06754491\r5=1.5258795\r6=1.52587489\r7=1.52596923\a5=102.15226041\a6=102.1410  
6407\a7=99.04340637\d5=60.49609499\d6=-  
60.18983276\d7=180.15118298\r8=1.5258708\r9=1.52588043\r10=1.52596878\a8=102.  
13676285\a9=102.15822858\a10=99.04042146\d8=240.15250067\d9=119.46472118\d1  
0=-0.18843236\Version=IA64L-G09RevA.02\State=1-A\HF=-  
4233.1293856\RMSD=7.717e-09\RMSF=4.032e-05\Dipole=-0.4045316,0.000624,-  
0.1855852\Quadrupole=-0.1746108,-5.820196,5.9948069,-0.0023933,-3.5883979,-  
0.0013417\PG=C01 [X(Ge2H7O1)]\@\
```

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge2H7O1(1+)\ROSMUS\18-Dec-2012\0\#\#p  
hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Ge,1,1.9258679451\Ge,1,1.9258596081,2,130.69072378\H,1,  
0.9647670359,2,114.63855286,3,180.06754491,0\H,2,1.525879501,1,102.15226041,4,60  
.49609499,0\H,2,1.5258748893,1,102.14106407,4,-
```

60.18983276,0\H,2,1.5259692264,1,99.04340637,4,180.15118298,0\H,3,1.5258708045,1  
,102.13676285,2,240.15250067,0\H,3,1.5258804301,1,102.15822858,2,119.46472118,0\  
H,3,1.5259687757,1,99.04042146,2,-0.18843236,0\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-4229.5829484\RMSD=5.157e-09\Dipole=-  
0.4060856,0.0006486,-0.186288\Quadrupole=-0.1580194,-5.8206405,5.9786599,-  
0.0023232,-3.5693993,-0.0012752\PG=C01 [X(Ge2H7O1)]\\@

HF=-4233.1293856

Sum of electronic and zero-point Energies= -4233.065928  
Sum of electronic and thermal Energies= -4233.059089  
Sum of electronic and thermal Enthalpies= -4233.058145  
Sum of electronic and thermal Free Energies= -4233.097914  
NImag=0

H3O3(1+)

-----  
1,1  
O  
O,1,r2  
O,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.40439475  
r3=1.40421875  
r4=0.99004596  
r5=0.97862766  
r6=0.97860645  
a3=110.01627888  
a4=103.70814737  
a5=102.00838039  
a6=102.02686559  
d4=110.39920111  
d5=220.04310367  
d6=250.63286668

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O3(1+)\ROSMUS\11-Dec-  
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\title\\1,1\O\O,1,r2\O,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6  
,0\r2=1.40439475\r3=1.40421875\r4=0.99004596\r5=0.97862766\r6=0.97860645\a3=11  
0.01627888\a4=103.70814737\a5=102.00838039\a6=102.02686559\d4=110.39920111\d  
5=220.04310367\d6=250.63286668\\Version=IA64L-G09RevA.02\State=1-A\HF=-

226.9347708\RMSD=5.358e-09\RMSF=1.102e-04\Dipole=-0.6418404,0.5811099,-  
0.4475584\Quadrupole=-1.094277,0.7121616,0.3821155,1.7046156,-  
2.0525529,1.1933678\PG=C01 [X(H3O3)]\ \@  
--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O3(1+)\ROSMUS\18-Dec-2012\0\#p hf  
cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\O,1,1.4043947451\O,1,1.4042187542,2,110.01627888\H,1,0.  
9900459642,2,103.70814737,3,110.39920111,0\H,2,0.9786276572,1,102.00838039,4,22  
0.04310367,0\H,3,0.9786064539,1,102.02686559,2,250.63286668,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-225.9111157\RMSD=6.688e-09\Dipole=-  
0.6262837,0.6236743,-0.4363763\Quadrupole=-  
1.1471638,0.7658248,0.381339,1.7372394,-2.1245413,1.216174\PG=C01  
[X(H3O3)]\ \@

HF=-226.9347708

Sum of electronic and zero-point Energies=	-226.890576
Sum of electronic and thermal Energies=	-226.886607
Sum of electronic and thermal Enthalpies=	-226.885663
Sum of electronic and thermal Free Energies=	-226.915628
NImag=0	

H3O1Se2(1+)

-----

1,1  
O  
Se,1,r2  
Se,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.88931862  
r3=1.8893164  
r4=0.96929061  
r5=1.47087988  
r6=1.47087886  
a3=127.14471136  
a4=115.10992566  
a5=91.40912192  
a6=91.40861066  
d4=160.55868134  
d5=259.77248408  
d6=260.81290635

--- Geometry Optimization ---

```
1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O1Se2(1+)\ROSMUS\11-  
Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Se,1,r2\Se,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,  
d6,0\r2=1.88931862\r3=1.8893164\r4=0.96929061\r5=1.47087988\r6=1.47087886\a3=1  
27.14471136\a4=115.10992566\a5=91.40912192\a6=91.40861066\d4=160.55868134\d5  
=259.77248408\d6=260.81290635\Version=IA64L-G09RevA.02\State=1-A\HF=-  
4879.7733419\RMSD=9.697e-09\RMSF=5.521e-05\Dipole=-0.5827638,0.4447292,-  
0.2895754\Quadrupole=-1.7627576,-2.851308,4.6140656,0.4302611,-  
4.2102465,0.2143482\PG=C01 [X(H3O1Se2)]\@
```

--- NBO Single Point ---

```
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O1Se2(1+)\ROSMUS\18-Dec-2012\0\#p  
hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Se,1,1.8893186195\Se,1,1.8893163971,2,127.14471136\H,1,0  
.9692906137,2,115.10992566,3,160.55868134,0\H,2,1.4708798802,1,91.40912192,4,259  
.77248408,0\H,3,1.4708788634,1,91.40861066,2,260.81290635,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-4876.0957946\RMSD=6.050e-09\Dipole=-  
0.579794,0.4659564,-0.2880879\Quadrupole=-1.8000285,-  
2.7435779,4.5436064,0.442534,-4.1884004,0.2204722\PG=C01 [X(H3O1Se2)]\@
```

HF=-4879.7733419

Sum of electronic and zero-point Energies=	-4879.741455
Sum of electronic and thermal Energies=	-4879.736355
Sum of electronic and thermal Enthalpies=	-4879.735410
Sum of electronic and thermal Free Energies=	-4879.771524
NImag=	0

H7O1Si2(1+)

```
-----  
1,1  
O  
Si,1,r2  
Si,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0
```

```
r2=1.7930554  
r3=1.79305202  
r4=0.96866254
```



a3=130.66962692  
a4=114.66456247  
d4=179.31858797  
r5=1.4613071  
r6=1.4618916  
r7=1.46063665  
a5=103.920607  
a6=103.14846084  
a7=100.77391089  
d5=65.18771824  
d6=-55.06652873  
d7=185.10729075  
r8=1.46185688  
r9=1.46134194  
r10=1.46064148  
a8=103.16698634  
a9=103.90212924  
a10=100.77584253  
d8=234.72064214  
d9=114.46934101  
d10=-5.4506194

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H7O1Si2(1+)\ROSMUS\13-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Si,1,r2\Si,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\|r2=1.7930554\r3=1.79305202\r4=0.96866254\|a3=130.66962692\|a4=114.66456247\|d4=179.31858797\|r5=1.4613071\|r6=1.4618916\|r7=1.46063665\|a5=103.920607\|a6=103.14846084\|a7=100.77391089\|d5=65.18771824\|d6=-55.06652873\|d7=185.10729075\|r8=1.46185688\|r9=1.46134194\|r10=1.46064148\|a8=103.16698634\|a9=103.90212924\|a10=100.77584253\|d8=234.72064214\|d9=114.46934101\|d10=-5.4506194\|Version=IA64L-G09RevA.02\|State=1-A\|HF=-658.1560208\|RMSD=7.446e-09\|RMSF=1.904e-05\|Dipole=-0.4295574,-0.0071369,-0.1972408\|Quadrupole=0.3015092,-4.9335455,4.6320364,0.0446912,-2.5204073,0.0212616\|PG=C01 [X(H7O1Si2)]\|@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H7O1Si2(1+)\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Si,1,1.7930554031\|Si,1,1.7930520236,2,130.66962692\|H,1,0.9686625392,2,114.66456247,3,179.31858797,0\|H,2,1.4613071047,1,103.920607,4,65.18771824,0\|H,2,1.4618915974,1,103.14846084,4,-55.06652873,0\|H,2,1.460636653,1,100.77391089,4,185.10729075,0\|H,3,1.4618568799,1,103.16698634,2,234.72064214,0\|H,3,1.4613419424,1,103.90212924,2,114.46934101,0\|H,3,1.4606414776,1,100.77584253,2,-5.4506194,0\|Version=IA64L-G09RevA.02\|State=1-A\|HF=-656.6841133\|RMSD=2.497e-09\|Dipole=-0.447607,-

0.0078802,-0.2055247\Quadrupole=0.3419271,-4.9354717,4.5935446,0.0490306,-  
2.4744281,0.0230495\PG=C01 [X(H7O1Si2)]\ \@

HF=-658.1560208

Sum of electronic and zero-point Energies= -658.088609  
Sum of electronic and thermal Energies= -658.082153  
Sum of electronic and thermal Enthalpies= -658.081208  
Sum of electronic and thermal Free Energies= -658.119051  
NImag=0

H3O1S2(1+)

-----  
1,1  
O  
S,1,r2  
S,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0

r2=1.73354909  
r3=1.73376367  
r4=0.97330017  
r5=1.34481374  
r6=1.3448106  
a3=126.5781232  
a4=116.57320251  
a5=93.62775219  
a6=93.6316763  
d4=186.32884986  
d5=269.86971863  
d6=276.42752882

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O1S2(1+)\ROSMUS\11-  
Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\S,1,r2\S,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,  
0\r2=1.73354909\r3=1.73376367\r4=0.97330017\r5=1.34481374\r6=1.3448106\a3=126.  
5781232\a4=116.57320251\a5=93.62775219\a6=93.6316763\d4=186.32884986\d5=269.  
86971863\d6=276.42752882\Version=IA64L-G09RevA.02\State=1-A\HF=-  
873.0177247\RMSD=9.735e-09\RMSF=2.640e-04\Dipole=-0.4870716,0.7564155,-  
0.2454891\Quadrupole=-0.7678018,-2.0341587,2.8019605,0.8150361,-  
2.4054928,0.4091318\PG=C01 [X(H3O1S2)]\ \@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O1S2(1+)\ROSMUS\18-Dec-2012\0\#p hf  
cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\S,1,1.7335490871\S,1,1.733763675,2,126.5781232\H,1,0.973  
300169,2,116.57320251,3,186.32884986,0\H,2,1.3448137388,1,93.62775219,4,269.8697  
1863,0\H,3,1.344810603,1,93.6316763,2,276.42752882,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-871.3905338\RMSD=2.749e-09\Dipole=-  
0.4802948,0.8165516,-0.242244\Quadrupole=-0.7980173,-  
1.9444277,2.742445,0.8681135,-2.3857431,0.4357814\PG=C01 [X(H3O1S2)]\@

HF=-873.0177247

Sum of electronic and zero-point Energies= -872.982996  
Sum of electronic and thermal Energies= -872.978349  
Sum of electronic and thermal Enthalpies= -872.977404  
Sum of electronic and thermal Free Energies= -873.010415  
NImag=0

Br3O1(1+)

-----  
1,1  
O  
Br,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.88474359  
r3=0.9779143  
r4=0.9779143  
a3=111.81563604  
a4=111.81563604  
d4=124.59391399

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Br1H2O1(1+)\ROSMUS\26-  
Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Br,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.88474359\r3=0.9779143\r4  
=0.9779143\a3=111.81563604\a4=111.81563604\d4=124.59391399\Version=IA64L-  
G09RevA.02\State=1-A\HF=-2650.2067769\RMSD=6.768e-09\RMSF=6.525e-  
05\Dipole=0.2855191,-0.5437636,-1.702869\Quadrupole=-2.5875318,-  
3.8562229,6.4437548,0.9197452,-1.2346691,2.3513947\PG=CS [SG(Br1O1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br3O1(1+)\ROSMUS\18-Dec-2012\0\#p hf  
cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Br,1,1.8797368833\Br,1,1.8776505302,2,114.64369789\Br,1,  
1.8790070993,2,113.99534384,3,135.05410135,0\Version=IA64L-

G09RevA.02\State=1-A\HF=-7791.7951708\RMSD=2.690e-09\Dipole=0.0720814,-  
0.1778782,0.0497779\Quadrupole=2.2668959,-5.4242205,3.1573246,3.8692592,-  
1.0737792,2.4466173\PG=C01 [X(Br3O1)]\@

HF=-2650.2067769

Sum of electronic and zero-point Energies= -2650.181198  
Sum of electronic and thermal Energies= -2650.178062  
Sum of electronic and thermal Enthalpies= -2650.177118  
Sum of electronic and thermal Free Energies= -2650.205865  
NImag=0

C3H9O1(1+)

-----  
1,1  
O  
C,1,r2  
C,1,r3,2,a3  
C,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0  
H,4,r11,1,a11,3,d11,0  
H,4,r12,1,a12,3,d12,0  
H,4,r13,1,a13,3,d13,0

r2=1.46414689  
r3=1.46423125  
r4=1.46399022  
a3=113.58964126  
a4=113.55346392  
d4=131.64487787  
r5=1.08892391  
r6=1.08471714  
r7=1.08463453  
a5=108.52551872  
a6=106.45058912  
a7=106.50913906  
d5=66.12750917  
d6=-54.60254055  
d7=186.88220882  
r8=1.08472487

r9=1.08887093  
r10=1.08466119  
a8=106.47694582  
a9=108.50054105  
a10=106.47757674  
d8=186.85008273  
d9=66.11188496  
d10=-54.62120082  
r11=1.08887273  
r12=1.08473024  
r13=1.08472499  
a11=108.48728539  
a12=106.4608708  
a13=106.494697  
d11=65.20202523  
d12=-55.51763955  
d13=185.91015539

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C3H9O1(1+)\ROSMUS\14-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\C,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.46414689\r3=1.46423125\r4=1.46399022\a3=113.58964126\a4=113.55346392\d4=131.64487787\r5=1.08892391\r6=1.08471714\r7=1.08463453\a5=108.52551872\a6=106.45058912\a7=106.50913906\d5=66.12750917\d6=-54.60254055\d7=186.88220882\r8=1.08472487\r9=1.08887093\r10=1.08466119\a8=106.47694582\a9=108.50054105\a10=106.47757674\d8=186.85008273\d9=66.11188496\d10=-54.62120082\r11=1.08887273\r12=1.08473024\r13=1.08472499\a11=108.48728539\a12=106.4608708\a13=106.494697\d11=65.20202523\d12=-55.51763955\d13=185.91015539\\Version=IA64L-G09RevA.02\State=1-A\HF=-194.6234699\RMSD=6.494e-09\RMSF=1.032e-04\Dipole=0.0851898,-0.1891804,0.0557983\Quadrupole=0.9368004,-2.3539668,1.4171664,1.8503024,-0.54752,1.2096754\PG=C01 [X(C3H9O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C3H9O1(1+)\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\C,1,1.464146888\C,1,1.4642312521,2,113.58964126\C,1,1.4639902224,2,113.55346392,3,131.64487787,0\H,2,1.08892391,1,108.52551872,4,66.12750917,0\H,2,1.0847171413,1,106.45058912,4,-54.60254055,0\H,2,1.0846345279,1,106.50913906,4,186.88220882,0\H,3,1.084724869,1,106.47694582,2,186.85008273,0\H,3,1.088870931,1,108.50054105,2,66.11188496,0\H,3,1.0846611904,1,106.47757674,2,-54.62120082,0\H,4,1.0888727344,1,108.48728539,3,65.20202523,0\H,4,1.0847302422,1

,106.4608708,3,-  
55.51763955,0\H,4,1.0847249892,1,106.494697,3,185.91015539,0\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-193.5105666\RMSD=5.443e-09\Dipole=0.0946129,-  
0.2100689,0.062024\Quadrupole=0.9192604,-2.3102387,1.3909783,1.8158992,-  
0.53734,1.1876175\PG=C01 [X(C3H9O1)]\@

HF=-194.6234699

Sum of electronic and zero-point Energies= -194.500793  
Sum of electronic and thermal Energies= -194.495093  
Sum of electronic and thermal Enthalpies= -194.494149  
Sum of electronic and thermal Free Energies= -194.528518  
NImag=0

Cl3O1(1+)

-----  
1,1  
O  
Cl,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.71802108  
r3=0.98195449  
r4=0.98195449  
a3=110.85634587  
a4=110.85634587  
d4=124.03962512

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Cl1H2O1(1+)\ROSMUS\26-  
Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Cl,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.71802108\r3=0.98195449\r  
4=0.98195449\a3=110.85634587\a4=110.85634587\d4=124.03962512\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-536.2100131\RMSD=5.250e-09\RMSF=1.382e-  
04\Dipole=0.2972182,-0.5594528,-1.3853346\Quadrupole=-1.5214548,-  
2.8119534,4.3334081,0.9551958,-1.0235699,1.9266619\PG=CS [SG(Cl1O1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl3O1(1+)\ROSMUS\18-Dec-2012\0\#p hf  
cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Cl,1,1.7220328132\Cl,1,1.7224441297,2,113.10657797\Cl,1,  
1.7224440604,2,113.10653547,3,130.26525631,0\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-1452.8925937\RMSD=5.149e-09\Dipole=0.0699969,-  
0.1510201,0.045617\Quadrupole=1.4329278,-3.6407025,2.2077747,2.9949907,-  
0.9162013,1.9767249\PG=C01 [X(Cl3O1)]\@

HF=-1455.2508818

Sum of electronic and zero-point Energies= -1455.244687  
Sum of electronic and thermal Energies= -1455.239993  
Sum of electronic and thermal Enthalpies= -1455.239048  
Sum of electronic and thermal Free Energies= -1455.274072  
NImag=0

F3O1(1+)

-----

1,1  
O  
F,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.37013943  
r3=0.99366816  
r4=0.99366816  
a3=105.32548592  
a4=105.32548592  
d4=119.02434528

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\F1H2O1(1+)\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\F,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.37013943\r3=0.99366816\r4=0.99366816\a3=105.32548592\a4=105.32548592\d4=119.02434528\Version=IA64L-G09RevA.02\State=1-A\HF=-175.7597544\RMSD=1.468e-09\RMSF=7.009e-05\Dipole=0.3944275,-0.6699304,-1.3333429\Quadrupole=0.0273944,-1.0859972,1.0586027,1.0033001,-0.7913212,1.3440498\PG=CS [SG(F1O1),X(H2)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F3O1(1+)\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\F,1,1.3501937182\F,1,1.3505166907,2,104.83887364\F,1,1.350516689,2,104.83886962,3,110.12562787,0\Version=IA64L-G09RevA.02\State=1-A\HF=-372.4923533\RMSD=6.773e-09\Dipole=-0.08631,0.1235516,-0.0664175\Quadrupole=0.1125387,-0.4381115,0.3255728,0.7513198,-0.4039996,0.5783195\PG=C01 [X(F3O1)]\@\

HF=-373.9199322

Sum of electronic and zero-point Energies= -373.909291  
Sum of electronic and thermal Energies= -373.905748

Sum of electronic and thermal Enthalpies= -373.904804  
Sum of electronic and thermal Free Energies= -373.935451  
NImag=0

Ge3H9O1(1+)

-----  
1,1  
O  
Ge,1,r2  
Ge,1,r3,2,a3  
Ge,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0  
H,4,r11,1,a11,3,d11,0  
H,4,r12,1,a12,3,d12,0  
H,4,r13,1,a13,3,d13,0

r2=1.8923342  
r3=1.89228744  
r4=1.89228318  
a3=119.97867499  
a4=120.00924764  
d4=179.97422932  
r5=1.52849981  
r6=1.53119952  
r7=1.52849613  
a5=103.42841002  
a6=100.77152166  
a7=103.42272313  
d5=119.52216119  
d6=-0.23260827  
d7=240.01961766  
r8=1.52870965  
r9=1.52869552  
r10=1.53131515  
a8=103.443798  
a9=103.46222089  
a10=100.69624828  
d8=240.04079478  
d9=119.55463299  
d10=-0.20322735



r11=1.52861001  
r12=1.53120963  
r13=1.52859393  
a11=103.44929102  
a12=100.78295872  
a13=103.4726314  
d11=120.40660906  
d12=0.60124582  
d13=240.8047758

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Ge3H9O1(1+)\ROSMUS\17-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(calcfc,z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Ge,1,r2\Ge,1,r3,2,a3\Ge,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.8923342\r3=1.89228744\r4=1.89228318\ a3=119.97867499\ a4=120.00924764\ d4=179.97422932\r5=1.52849981\r6=1.53119952\r7=1.52849613\ a5=103.42841002\ a6=100.77152166\ a7=103.42272313\ d5=119.52216119\ d6=-0.23260827\ d7=240.01961766\ r8=1.52870965\ r9=1.52869552\ r10=1.53131515\ a8=103.443798\ a9=103.46222089\ a10=100.69624828\ d8=240.04079478\ d9=119.55463299\ d10=-

0.20322735\r11=1.52861001\r12=1.53120963\r13=1.52859393\ a11=103.44929102\ a12=100.78295872\ a13=103.4726314\ d11=120.40660906\ d12=0.60124582\ d13=240.8047758\ \Version=IA64L-G09RevA.02\State=1-A\HF=-6311.3274686\RMSD=1.656e-09\RMSF=5.756e-05\Dipole=0.0011724,-0.0002873,-0.001011\Quadrupole=3.4104462,-6.8279,3.4174539,0.0042176,0.0002799,0.0010689\PG=C01 [X(Ge3H9O1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge3H9O1(1+)\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Ge,1,1.8923342029\Ge,1,1.8922874421,2,119.97867499\Ge,1,1.8922831813,2,120.00924764,3,179.97422932,0\H,2,1.5284998075,1,103.42841002,4,119.52216119,0\H,2,1.531199521,1,100.77152166,4,-0.23260827,0\H,2,1.5284961274,1,103.42272313,4,240.01961766,0\H,3,1.5287096513,1,103.443798,2,240.04079478,0\H,3,1.5286955186,1,103.46222089,2,119.55463299,0\H,3,1.53131515,1,100.69624828,2,-0.20322735,0\H,4,1.5286100064,1,103.44929102,3,120.40660906,0\H,4,1.5312096285,1,100.78295872,3,0.60124582,0\H,4,1.5285939319,1,103.4726314,3,240.8047758,0\Version=IA64L-G09RevA.02\State=1-A\HF=-6306.1788588\RMSD=2.707e-09\Dipole=0.0014666,-0.0003229,-0.0005078\Quadrupole=3.3826405,-6.7724964,3.3898559,0.0041984,-0.000454,0.0009137\PG=C01 [X(Ge3H9O1)]\@\

HF=-6311.3274686

Sum of electronic and zero-point Energies= -6311.250737  
Sum of electronic and thermal Energies= -6311.241175

Sum of electronic and thermal Enthalpies= -6311.240231  
Sum of electronic and thermal Free Energies= -6311.288392  
NImag=0

H3O4(1+)

-----  
1,1  
O  
O,1,r2  
O,1,r3,2,a3  
O,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0  
H,4,r7,1,a7,3,d7,0

r2=1.40093147  
r3=1.40118994  
r4=1.40098568  
r5=0.98125731  
r6=0.98138344  
r7=0.98122194  
a3=105.49234189  
a4=105.50491593  
a5=101.66035331  
a6=101.68298397  
a7=101.63730065  
d4=111.45690626  
d5=203.88873132  
d6=203.29574923  
d7=204.32250754

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O4(1+)\ROSMUS\14-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\O,1,r2\O,1,r3,2,a3\O,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\H,4,r7,1,a7,3,d7,0\r2=1.40093147\r3=1.40118994\r4=1.40098568\r5=0.98125731\r6=0.98138344\r7=0.98122194\a3=105.49234189\a4=105.50491593\a5=101.66035331\a6=101.68298397\a7=101.63730065\d4=111.45690626\d5=203.88873132\d6=203.29574923\d7=204.32250754\Version=IA64L-G09RevA.02\State=1-A\HF=-302.0627374\RMSD=3.087e-09\RMSF=9.728e-05\Dipole=-0.7433407,1.0870878,-0.5728903\Quadrupole=0.3778436,-1.459612,1.0817684,2.2873644,-1.1838731,1.7827041\PG=C01 [X(H3O4)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O4(1+)\ROSMUS\18-Dec-2012\0\#\#p hf cc-pvqz scf=verytight guess=read geom=allcheck

pop=savenbos\\title\\1,1\O\O,1,1.4009314701\O,1,1.4011899358,2,105.49234189\O,1,1.4009856767,2,105.50491593,3,111.45690626,0\H,2,0.9812573103,1,101.66035331,4,203.88873132,0\H,3,0.9813834412,1,101.68298397,2,203.29574923,0\H,4,0.9812219354,1,101.63730065,3,204.32250754,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-300.7008256\RMSD=6.114e-09\Dipole=-0.7654573,1.119584,-0.5903994\Quadrupole=0.3842033,-1.4829801,1.0987768,2.3221565,-1.2024198,1.8103295\PG=C01 [X(H3O4)]\\@

HF=-302.0627374

Sum of electronic and zero-point Energies= -302.016030  
Sum of electronic and thermal Energies= -302.010875  
Sum of electronic and thermal Enthalpies= -302.009931  
Sum of electronic and thermal Free Energies= -302.043274  
NImag=0

H3O1Se3(1+)

-----  
1,1  
O  
X,1,1.  
Se,1,rS,2,aS  
Se,1,rS,2,aS,3,dS,0  
Se,1,rS,2,aS,3,-dS,0  
H,3,rH,1,aH,2,dH,0  
H,4,rH,1,aH,2,dH,0  
H,5,rH,1,aH,2,dH,0

rS=1.88873695  
rH=1.47189767  
aS=90.9647781  
aH=92.20985076  
dS=120.  
dH=180.

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O1Se3(1+)\ROSMUS\14-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\title\\1,1\O\X,1,1.\Se,1,rS,2,aS\Se,1,rS,2,aS,3,dS,0\Se,1,rS,2,aS,3,-dS,0\H,3,rH,1,aH,2,dH,0\H,4,rH,1,aH,2,dH,0\H,5,rH,1,aH,2,dH,0\\rS=1.88873695\rH=1.47189767\aS=90.9647781\aH=92.20985076\dS=120.\dH=180.\\Version=IA64L-G09RevA.02\State=1-A1\HF=-7281.304168\RMSD=5.613e-09\RMSF=1.167e-05\Dipole=0.,0.,-0.877858\Quadrupole=1.428931,1.428931,-2.857862,0.,0.,0.\PG=C03V [C3(O1),3SGV(H1Se1)]\\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O1Se3(1+)\ROSMUS\18-Dec-2012\0\#p  
hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\X,1,1.\Se,1,1.8887369474,2,90.9647781\Se,1,1.8887369474,2  
,90.9647781,3,120.,0\Se,1,1.8887369474,2,90.9647781,3,-  
120.,0\H,3,1.4718976691,1,92.20985076,2,180.,0\H,4,1.4718976691,1,92.20985076,2,18  
0.,0\H,5,1.4718976691,1,92.20985076,2,180.,0\Version=IA64L-G09RevA.02\State=1-  
A1\HF=-7275.9574719\RMSD=5.436e-09\Dipole=0.,0.,-  
0.9179846\Quadrupole=1.3236534,1.3236534,-2.6473067,0.,0.,0.\PG=C03V  
[C3(O1),3SGV(H1Se1)]\@

HF=-7281.304168

Sum of electronic and zero-point Energies= -7281.276229  
Sum of electronic and thermal Energies= -7281.268253  
Sum of electronic and thermal Enthalpies= -7281.267309  
Sum of electronic and thermal Free Energies= -7281.311754  
NImag=0

H9O1Si3(1+)

-----  
1,1  
O  
Si,1,r2  
Si,1,r3,2,a3  
Si,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0  
H,3,r8,1,a8,2,d8,0  
H,3,r9,1,a9,2,d9,0  
H,3,r10,1,a10,2,d10,0  
H,4,r11,1,a11,3,d11,0  
H,4,r12,1,a12,3,d12,0  
H,4,r13,1,a13,3,d13,0

r2=1.77013188  
r3=1.76974438  
r4=1.76980484  
a3=119.95864974  
a4=120.03953488  
d4=179.98543224  
r5=1.4633347  
r6=1.46606574  
r7=1.46334243  
a5=104.6828609

a6=101.63586605  
a7=104.68124267  
d5=119.6378911  
d6=0.0245962  
d7=240.4093702  
r8=1.46289875  
r9=1.46289567  
r10=1.46587795  
a8=104.6868327  
a9=104.69215159  
a10=101.52119527  
d8=240.458173  
d9=119.61923196  
d10=0.04042822  
r11=1.46290692  
r12=1.46618169  
r13=1.46292814  
a11=104.70967114  
a12=101.5795333  
a13=104.71272148  
d11=119.52054829  
d12=-0.10351426  
d13=240.27505993

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H9O1Si3(1+)\ROSMUS\14-Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Si,1,r2\Si,1,r3,2,a3\Si,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\H,3,r8,1,a8,2,d8,0\H,3,r9,1,a9,2,d9,0\H,3,r10,1,a10,2,d10,0\H,4,r11,1,a11,3,d11,0\H,4,r12,1,a12,3,d12,0\H,4,r13,1,a13,3,d13,0\r2=1.77013188\r3=1.76974438\r4=1.76980484\a3=119.95864974\a4=120.03953488\d4=179.98543224\r5=1.4633347\r6=1.46606574\r7=1.46334243\a5=104.6828609\a6=101.63586605\a7=104.68124267\d5=119.6378911\d6=0.0245962\d7=240.4093702\r8=1.46289875\r9=1.46289567\r10=1.46587795\a8=104.6868327\a9=104.69215159\a10=101.52119527\d8=240.458173\d9=119.61923196\d10=0.04042822\r11=1.46290692\r12=1.46618169\r13=1.46292814\a11=104.70967114\a12=101.5795333\a13=104.71272148\d11=119.52054829\d12=-0.10351426\d13=240.27505993\\Version=IA64L-G09RevA.02\State=1-A\HF=-948.8781989\RMSD=9.658e-09\RMSF=8.496e-05\Dipole=0.0000114,-0.0000365,0.0001715\Quadrupole=2.8328474,-5.6697936,2.8369462,0.0006753,0.0016913,0.0007358\PG=C01 [X(H9O1Si3)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H9O1Si3(1+)\ROSMUS\18-Dec-2012\0\#p hf cc-pvqz scf=verytight guess=read geom=allcheck  
pop=savenbos\title\1,1\O\Si,1,1.7701318815\Si,1,1.7697443822,2,119.95864974\Si,1,1.7698048404,2,120.03953488,3,179.98543224,0\H,2,1.463334696,1,104.6828609,4,119.6378911,0\H,2,1.4660657431,1,101.63586605,4,0.0245962,0\H,2,1.4633424285,1,104.68

124267,4,240.4093702,0\H,3,1.4628987514,1,104.6868327,2,240.458173,0\H,3,1.46289  
56739,1,104.69215159,2,119.61923196,0\H,3,1.4658779538,1,101.52119527,2,0.040428  
22,0\H,4,1.4629069154,1,104.70967114,3,119.52054829,0\H,4,1.466181687,1,101.5795  
333,3,-  
0.10351426,0\H,4,1.4629281405,1,104.71272148,3,240.27505993,0\\Version=IA64L-  
G09RevA.02\State=1-A\HF=-946.8409591\RMSD=9.515e-09\Dipole=0.0003578,-  
0.0000411,-0.0010105\Quadrupole=2.8214533,-5.6469175,2.8254642,0.0006395,-  
0.0008276,0.0007901\PG=C01 [X(H9O1Si3)]\@\@

HF=-948.8781989

Sum of electronic and zero-point Energies= -948.794729  
Sum of electronic and thermal Energies= -948.786391  
Sum of electronic and thermal Enthalpies= -948.785447  
Sum of electronic and thermal Free Energies= -948.827963  
NImag=0

H3O1S3(1+)

-----  
1,1  
O  
S,1,r2  
S,1,r3,2,a3  
S,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,3,r6,1,a6,2,d6,0  
H,4,r7,1,a7,3,d7,0

r2=1.74125266  
r3=1.74178348  
r4=1.74143727  
r5=1.34446521  
r6=1.34444566  
r7=1.344564  
a3=119.97127894  
a4=120.03108581  
a5=93.55613284  
a6=93.46163183  
a7=93.57263063  
d4=181.83434307  
d5=269.9233388  
d6=270.97915707  
d7=271.29456209

--- Geometry Optimization ---

```

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O1S3(1+)\ROSMUS\17-
Dec-2012\1\#p m062x 6-311++G(3df,2p) opt=(calcfc,z-matrix,noeigen) optcyc=100
freq\title\1,1\O\S,1,r2\S,1,r3,2,a3\S,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,
0\H,4,r7,1,a7,3,d7,0\r2=1.74125266\r3=1.74178348\r4=1.74143727\r5=1.34446521\r6=
1.34444566\r7=1.344564\ a3=119.97127894\ a4=120.03108581\ a5=93.55613284\ a6=93.4
6163183\ a7=93.57263063\ d4=181.83434307\ d5=269.9233388\ d6=270.97915707\ d7=27
1.29456209\Version=IA64L-G09RevA.02\State=1-A\HF=-
1271.1763255\RMSD=7.683e-09\RMSF=8.960e-
05\Dipole=0.0239881,1.0221216,0.0072822\Quadrupole=0.8334736,-
1.6860953,0.8526217,0.0098986,0.0372944,-0.0339587\PG=C01 [X(H3O1S3)]\@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O1S3(1+)\ROSMUS\18-Dec-2012\0\#p hf
cc-pvqz scf=verytight guess=read geom=allcheck
pop=savenbos\title\1,1\O\S,1,1.7412526636\S,1,1.7417834753,2,119.97127894\S,1,1.7
414372748,2,120.03108581,3,181.83434307,0\H,2,1.3444652069,1,93.55613284,4,269.9
233388,0\H,3,1.3444456616,1,93.46163183,2,270.97915707,0\H,4,1.3445639989,1,93.5
7263063,3,271.29456209,0\Version=IA64L-G09RevA.02\State=1-A\HF=-
1268.9059066\RMSD=9.384e-
09\Dipole=0.0254867,1.1094626,0.0078917\Quadrupole=0.7568015,-
1.5290558,0.7722543,0.0130564,0.0408397,-0.0330328\PG=C01 [X(H3O1S3)]\@

```

HF=-1271.1763255

```

Sum of electronic and zero-point Energies=      -1271.142869
Sum of electronic and thermal Energies=        -1271.136721
Sum of electronic and thermal Enthalpies=      -1271.135777
Sum of electronic and thermal Free Energies=    -1271.173325
NImag=0

```

H3P1S3

-----

```

0,1
P
S,1,r2
S,1,r3,2,a3
S,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,3,r6,1,a6,2,d6,0
H,4,r7,1,a7,3,d7,0

```

```

r2=2.11350157
r3=2.11400827
r4=2.11261891
r5=1.34164573
r6=1.34164093

```

r7=1.34166991  
a3=104.4836905  
a4=104.45430986  
a5=98.44080529  
a6=98.43692755  
a7=98.32881272  
d4=250.79134875  
d5=306.26463236  
d6=300.5243329  
d7=303.8361988

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3P1S3\ROSMUS\13-Dec-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\P\S,1,r2\S,1,r3,2,a3\S,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,3,r6,1,a6,2,d6,0\H,4,r7,1,a7,3,d7,0\r2=2.11350157\r3=2.11400827\r4=2.11261891\r5=1.34164573\r6=1.34164093\r7=1.34166991\a3=104.4836905\a4=104.45430986\a5=98.44080529\a6=98.43692755\a7=98.32881272\d4=250.79134875\d5=306.26463236\d6=300.5243329\d7=303.8361988\Version=IA64L-G09RevA.02\State=1-A\HF=-1537.7562808\RMSD=9.021e-09\RMSF=1.640e-04\Dipole=0.3983093,0.6043798,0.3061677\Quadrupole=-0.4720688,1.639385,-1.1673162,2.6005623,1.3359234,1.9773712\PG=C01 [X(H3P1S3)]\@\nbo  
--- NBO Single Point ---

HF=-1537.7562808

Sum of electronic and zero-point Energies= -1537.724541  
Sum of electronic and thermal Energies= -1537.718146  
Sum of electronic and thermal Enthalpies= -1537.717202  
Sum of electronic and thermal Free Energies= -1537.755588  
NImag=0

Br1H1S1

-----  
0,1  
S  
Br,1,r2  
H,1,r3,2,a3

r2=2.18528856  
r3=1.33947537  
a3=95.17427641

--- Geometry Optimization ---



```

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Br1H1S1\ROSMUS\26-Jul-
2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100
freq\title\0,1\S\Br,1,r2\H,1,r3,2,a3\r2=2.18528856\r3=1.33947537\a3=95.17427641\Version=IA64L-G09RevA.02\State=1-A\HF=-2972.9540612\RMSD=6.440e-
09\RMSF=2.204e-04\Dipole=0.3292653,0.,-0.2528979\Quadrupole=0.5909264,-
2.1540512,1.5631248,0.,-1.3030034,0.\PG=CS [SG(Br1H1S1)]\@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br1H1S1\ROSMUS\26-Jul-2012\0\#p hf/cc-
pvqz scf=verytight pop=(nboread) geom=allcheck
guess=read\title\0,1\S\Br,1,2.185288558\H,1,1.3394753702,2,95.17427641\Version=I
A64L-G09RevA.02\State=1-A\HF=-2970.5954555\RMSD=9.767e-
09\Dipole=0.3639101,0.,-0.2815309\Quadrupole=0.6316772,-2.1037522,1.472075,0.,-
1.4273479,0.\PG=CS [SG(Br1H1S1)]\@

```

HF=-2972.9540612

```

Sum of electronic and zero-point Energies=      -2972.944772
Sum of electronic and thermal Energies=      -2972.941619
Sum of electronic and thermal Enthalpies=      -2972.940675
Sum of electronic and thermal Free Energies=    -2972.970382
NImag=0

```

C1H4S1

```

-----
0,1
S
C,1,r2
X,1,1.,2,110.65
H,1,r4,2,a4,3,d4,0
H,2,r5,1,a5,4,d5,0
H,2,r6,1,a6,4,d6,0
H,2,r7,1,a7,4,d7,0

```

```

r2=1.81232813
r4=1.33719876
a4=96.961842
d4=88.16808273
r5=1.08597917
r6=1.08597918
r7=1.08710678
a5=111.21120611
a6=111.20995925
a7=106.16298087
d5=61.8193616
d6=-61.77407429

```

d7=180.02339258

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\C1H4S1\ROSMUS\23-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\S\C,1,r2\X,1,1.,2,110.65\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.81232813\r4=1.33719876\a4=96.961842\d4=88.16808273\r5=1.08597917\r6=1.08597918\r7=1.08710678\a5=111.21120611\a6=111.20995925\a7=106.16298087\d5=61.81936169\d6=-61.77407429\d7=180.02339258\Version=IA64L-G09RevA.02\State=1-A\HF=-438.684739\RMSD=6.793e-09\RMSF=1.211e-05\Dipole=0.0087314,-0.2733216,0.5477545\Quadrupole=-1.4148045,1.1343014,0.2805031,-0.0816149,-0.0287507,0.8972797\PG=C01 [X(C1H4S1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C1H4S1\ROSMUS\23-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\S\C,1,1.8123281346\X,1,1.,2,110.65\H,1,1.3371987588,2,96.961842,3,88.16808273,0\H,2,1.0859791707,1,111.21120611,4,61.81936169,0\H,2,1.0859791829,1,111.20995925,4,-61.77407429,0\H,2,1.0871067812,1,106.16298087,4,180.02339258,0\Version=IA64L-G09RevA.02\State=1-A\HF=-437.7640131\RMSD=6.166e-09\Dipole=0.0096052,-0.3006503,0.5808186\Quadrupole=-1.3776073,1.1602314,0.217376,-0.0812531,-0.0309335,0.9658397\PG=C01 [X(C1H4S1)]\@

HF=-438.684739

Sum of electronic and zero-point Energies=	-438.639107
Sum of electronic and thermal Energies=	-438.636004
Sum of electronic and thermal Enthalpies=	-438.635060
Sum of electronic and thermal Free Energies=	-438.662962
NImag=1	

Cl1H1S1

-----

0,1

S

Cl,1,r2

H,1,r3,2,a3

r2=2.02665742

r3=1.33877908

a3=95.62531652

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C11H1S1\ROSMUS\26-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\S\Cl,1,r2\H,1,r3,2,a3\r2=2.02665742\r3=1.33877908\a3=95.62531652\Version=IA64L-G09RevA.02\State=1-A\HF=-858.9746662\RMSD=8.541e-09\RMSF=2.148e-04\Dipole=0.3383642,0.,-0.323538\Quadrupole=0.8517793,-1.8320119,0.9802326,0.,-1.0185757,0.\PG=CS [SG(C11H1S1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C11H1S1\ROSMUS\26-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\S\Cl,1,2.0266574197\H,1,1.3387790768,2,95.62531652\Version=IA64L-G09RevA.02\State=1-A\HF=-857.6454482\RMSD=6.856e-09\Dipole=0.3724978,0.,-0.372417\Quadrupole=0.9208624,-1.7716131,0.8507507,0.,-1.1083484,0.\PG=CS [SG(C11H1S1)]\@\

HF=-858.9746662

Sum of electronic and zero-point Energies=	-858.965032
Sum of electronic and thermal Energies=	-858.961968
Sum of electronic and thermal Enthalpies=	-858.961024
Sum of electronic and thermal Free Energies=	-858.989448
NImag=0	

F1H1S1

-----

0,1  
S  
F,1,r2  
H,1,r3,2,a3

r2=1.61728606  
r3=1.33982521  
a3=95.5231756

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\F1H1S1\ROSMUS\23-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\S\F,1,r2\H,1,r3,2,a3\r2=1.61728606\r3=1.33982521\a3=95.5231756\Version=IA64L-G09RevA.02\State=1-A\HF=-498.5956191\RMSD=2.660e-09\RMSF=1.617e-04\Dipole=0.3453419,0.,-0.4584651\Quadrupole=1.3556738,-1.317289,-0.0383849,0.,-0.6749018,0.\PG=CS [SG(F1H1S1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F1H1S1\ROSMUS\23-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\S\F,1,1.6172860621\H,1,1.3398252137,2,95.5231756\Version=IA64L-G09RevA.02\State=1-A\HF=-497.5817075\RMSD=3.846e-

09\Dipole=0.3788007,0.,-0.551947\Quadrupole=1.41575,-1.275926,-0.139824,0.,-0.7453496,0.\PG=CS [SG(F1H1S1)]\@

HF=-498.5956191

Sum of electronic and zero-point Energies= -498.585178  
Sum of electronic and thermal Energies= -498.582243  
Sum of electronic and thermal Enthalpies= -498.581299  
Sum of electronic and thermal Free Energies= -498.608427  
NImag=0

Ge1H4S1

-----  
0,1  
S  
Ge,1,r2  
X,1,1.,2,110.65  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=2.23777793  
r4=1.33903679  
a4=94.38619911  
d4=252.01761264  
r5=1.53994759  
r6=1.54002249  
r7=1.53715638  
a5=109.99829745  
a6=110.03873802  
a7=104.84814949  
d5=60.1509598  
d6=-61.22938699  
d7=179.4924818

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Ge1H4S1\ROSMUS\26-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\S\Ge,1,r2\X,1,1.,2,110.65\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=2.23777793\r4=1.33903679\a4=94.38619911\d4=252.01761264\r5=1.53994759\r6=1.54002249\r7=1.53715638\a5=109.99829745\a6=110.03873802\a7=104.84814949\d5=60.1509598\d6=-61.22938699\d7=179.4924818\Version=IA64L-G09RevA.02\State=1-A\HF=-2477.5729025\RMSD=7.131e-09\RMSF=4.362e-05\Dipole=-

0.085548,0.2625467,0.472503\Quadrupole=-0.8226026,1.3692523,-0.5466497,-  
0.7952501,0.3996932,-1.2401616\PG=C01 [X(Ge1H4S1)]\@  
--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge1H4S1\ROSMUS\26-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\S\Ge,1,2.2377779346\X,1,1.,2,110.65\H,1,1.339036792,2,94.38619  
911,3,252.01761264,0\H,2,1.5399475864,1,109.99829745,4,60.1509598,0\H,2,1.540022  
4919,1,110.03873802,4,-  
61.22938699,0\H,2,1.5371563783,1,104.84814949,4,179.4924818,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-2475.3096531\RMSD=8.063e-09\Dipole=-  
0.0953482,0.2926986,0.4931036\Quadrupole=-0.7477724,1.4320788,-0.6843064,-  
0.7909222,0.430467,-1.3356235\PG=C01 [X(Ge1H4S1)]\@

HF=-2477.5729025

Sum of electronic and zero-point Energies=	-2477.540677
Sum of electronic and thermal Energies=	-2477.536883
Sum of electronic and thermal Enthalpies=	-2477.535939
Sum of electronic and thermal Free Energies=	-2477.567302

NImag=1

H3N1S1  
-----

--- Geometry Optimization ---

--- NBO Single Point ---  
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3N1S1\ROSMUS\20-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\S\N,1,1.7066090027\X,1,1.0154182,2,104.68557609\H,1,1.340069  
245,2,97.34109554,3,175.58481361,0\H,2,1.0101473649,1,111.06604867,4,241.4158506  
4,0\H,2,1.0101508335,1,111.05580957,4,118.82089227,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-453.7546872\RMSD=4.956e-  
09\Dipole=0.1806503,0.0149663,0.3757978\Quadrupole=0.2148307,-  
0.5531278,0.3382971,0.055674,2.6485341,0.2085354\PG=C01 [X(H3N1S1)]\@

HF=-454.7197605

Sum of electronic and zero-point Energies=	-454.684251
Sum of electronic and thermal Energies=	-454.680869
Sum of electronic and thermal Enthalpies=	-454.679925
Sum of electronic and thermal Free Energies=	-454.707995

NImag=0

H2O1S1

-----  
0,1  
S  
N,1,r2  
X,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0

r2=1.706609  
r4=1.34006925  
r5=1.01014736  
a4=97.34109554  
a5=111.06604867  
d4=175.58481361  
d5=241.41585064  
r6=1.01015083  
a6=111.05580957  
d6=118.82089227  
r3=1.0154182  
a3=104.68557609

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\H3N1S1\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\S\N,1,r2\X,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\r2=1.706609\r4=1.34006925\r5=1.01014736\a4=97.34109554\a5=111.06604867\d4=175.58481361\d5=241.41585064\r6=1.01015083\a6=111.05580957\d6=118.82089227\r3=1.0154182\a3=104.68557609\Version=IA64L-G09RevA.02\State=1-A\HF=-454.7197605\RMSD=4.210e-09\RMSF=5.752e-05\Dipole=0.1860323,0.0152979,0.3776335\Quadrupole=0.1384935,-0.5434563,0.4049628,0.0488908,2.5364959,0.1998685\PG=C01 [X(H3N1S1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H2O1S1\ROSMUS\20-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\S\O,1,1.6560775122\X,1,1.0154182,2,104.68557609\H,1,1.3433181508,2,98.31351871,3,152.15544087,0\H,2,0.9607924469,1,108.47158374,4,268.52200778,0\Version=IA64L-G09RevA.02\State=1-A\HF=-473.5844593\RMSD=2.781e-09\Dipole=-0.5724343,0.3726681,-0.0220474\Quadrupole=0.0840673,-0.2706756,0.1866083,0.5004542,-0.1783449,2.2019745\PG=C01 [X(H2O1S1)]\@

HF=-474.582755

Sum of electronic and zero-point Energies= -474.559818

Sum of electronic and thermal Energies= -474.556617  
Sum of electronic and thermal Enthalpies= -474.555673  
Sum of electronic and thermal Free Energies= -474.583304  
NImag=0

H4S1Si1

-----  
--- Geometry Optimization ---

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H4S1Si1\ROSMUS\26-Jul-2012\0\#p hf/cc-  
pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\0,1\Si,1,2.141380212\X,1,1.,2,110.65\H,1,1.3397948513,2,94.60206  
17,3,482.39621501,0\H,2,1.4740343293,1,111.19960438,4,60.45793114,0\H,2,1.474085  
7412,1,111.28041299,4,-  
61.43176173,0\H,2,1.4724583471,1,104.93897149,4,179.50180465,0\Version=IA64L-  
G09RevA.02\State=1-A\HF=-688.8560061\RMSD=3.695e-09\Dipole=-0.1756274,-  
0.276183,0.3408234\Quadrupole=-0.4375771,0.6870554,-  
0.2494783,1.1953112,0.630642,0.9916956\PG=C01 [X(H4S1Si1)]\@

HF=-690.0839426

Sum of electronic and zero-point Energies= -690.050124  
Sum of electronic and thermal Energies= -690.046519  
Sum of electronic and thermal Enthalpies= -690.045574  
Sum of electronic and thermal Free Energies= -690.075460  
NImag=1

Br1H2O1(1+)

-----  
0,1  
S  
Si,1,r2  
X,1,1.,2,110.65  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=2.14138021  
r4=1.33979485  
a4=94.6020617

d4=482.39621501  
r5=1.47403433  
r6=1.47408574  
r7=1.47245835  
a5=111.19960438  
a6=111.28041299  
a7=104.93897149  
d5=60.45793114  
d6=-61.43176173  
d7=179.50180465

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\H4S1Si1\ROSMUS\26-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\0,1\S\Si,1,r2\X,1,1.,2,110.65\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=2.14138021\r4=1.33979485\a4=94.6020617\d4=482.39621501\r5=1.47403433\r6=1.47408574\r7=1.47245835\a5=111.19960438\a6=111.28041299\a7=104.93897149\d5=60.45793114\d6=-61.43176173\d7=179.50180465\Version=IA64L-G09RevA.02\State=1-A\HF=-690.0839426\RMSD=8.047e-09\RMSF=4.492e-05\Dipole=-0.1592879,-0.2504681,0.3182115\Quadrupole=-0.5113079,0.6226947,-0.1113868,1.2054053,0.5867574,0.9230222\PG=C01 [X(H4S1Si1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Br1H2O1(1+)\ROSMUS\26-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\1,1\O\Br,1,1.884743593\H,1,0.9779142952,2,111.81563604\H,1,0.9779142952,2,111.81563604,3,124.59391399,0\Version=IA64L-G09RevA.02\State=1-A\HF=-2648.1629837\RMSD=4.520e-09\Dipole=0.293685,-0.5593154,-1.638649\Quadrupole=-2.5486671,-3.8061699,6.354837,0.9116341,-1.2501857,2.3809456\PG=CS [SG(Br1O1),X(H2)]\@

HF=-2650.2067769

Sum of electronic and zero-point Energies= -2650.181198  
Sum of electronic and thermal Energies= -2650.178062  
Sum of electronic and thermal Enthalpies= -2650.177118  
Sum of electronic and thermal Free Energies= -2650.205865  
NImag=0

C1H5O1(1+)

-----  
1,1  
O  
C,1,r2  
H,1,r3,2,a3



H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.49936216  
r3=0.97332789  
r4=0.97332923  
a3=114.82191757  
a4=114.82126046  
d4=129.92598134  
r5=1.08451503  
r6=1.08381536  
r7=1.08383166  
a5=108.39536544  
a6=104.80363902  
a7=104.80962131  
d5=64.92755184  
d6=-56.2464372  
d7=186.09749256

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\C1H5O1(1+)\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\C,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.49936216\r3=0.97332789\r4=0.97332923\a3=114.82191757\ a4=114.82126046\d4=129.92598134\r5=1.08451503\r6=1.08381536\r7=1.08383166\a5=108.39536544\a6=104.80363902\a7=104.80962131\d5=64.92755184\d6=-56.2464372\d7=186.09749256\Version=IA64L-G09RevA.02\State=1-A\HF=-116.0083646\RMSD=3.511e-09\RMSF=2.161e-05\Dipole=0.2127805,-0.4554864,-0.537279\Quadrupole=-0.2862969,-1.7643487,2.0506456,0.8829895,-0.6599998,1.413415\PG=C01 [X(C1H5O1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\C1H5O1(1+)\ROSMUS\20-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\1,1\O\C,1,1.4993621619\H,1,0.9733278896,2,114.82191757\H,1,0.9733292309,2,114.82126046,3,129.92598134,0\H,2,1.0845150349,1,108.39536544,4,64.92755184,0\H,2,1.0838153604,1,104.80363902,4,-56.2464372,0\H,2,1.0838316649,1,104.80962131,4,186.09749256,0\Version=IA64L-G09RevA.02\State=1-A\HF=-115.4061253\RMSD=9.312e-09\Dipole=0.2190108,-0.4688273,-0.5075628\Quadrupole=-0.2751801,-1.7496482,2.0248282,0.8808464,-0.6669785,1.4283487\PG=C01 [X(C1H5O1)]\@\

HF=-116.0083646

Sum of electronic and zero-point Energies= -115.943649

Sum of electronic and thermal Energies= -115.940039  
Sum of electronic and thermal Enthalpies= -115.939095  
Sum of electronic and thermal Free Energies= -115.966862  
NImag=0

Cl1H2O1(1+)

-----  
1,1  
O  
Cl,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.71802108  
r3=0.98195449  
r4=0.98195449  
a3=110.85634587  
a4=110.85634587  
d4=124.03962512

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\Cl1H2O1(1+)\ROSMUS\26-Jul-2012\1\#\p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Cl,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.71802108\r3=0.98195449\r4=0.98195449\ a3=110.85634587\ a4=110.85634587\ d4=124.03962512\Version=IA64L-G09RevA.02\State=1-A\HF=-536.2100131\RMSD=5.250e-09\RMSF=1.382e-04\Dipole=0.2972182,-0.5594528,-1.3853346\Quadrupole=-1.5214548,-2.8119534,4.3334081,0.9551958,-1.0235699,1.9266619\PG=CS [SG(Cl1O1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl1H2O1(1+)\ROSMUS\26-Jul-2012\0\#\p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\1,1\O\Cl,1,1.7180210757\H,1,0.9819544915,2,110.85634587\H,1,0.9819544915,2,110.85634587,3,124.03962512,0\Version=IA64L-G09RevA.02\State=1-A\HF=-535.1920086\RMSD=2.959e-09\Dipole=0.3066262,-0.5771614,-1.3432025\Quadrupole=-1.5100943,-2.7896494,4.2997437,0.9470957,-1.0352887,1.9487201\PG=CS [SG(Cl1O1),X(H2)]\@

HF=-536.2100131

Sum of electronic and zero-point Energies= -536.183961  
Sum of electronic and thermal Energies= -536.180921  
Sum of electronic and thermal Enthalpies= -536.179977  
Sum of electronic and thermal Free Energies= -536.207381  
NImag=0

F1H2O1(1+)

-----  
1,1  
O  
F,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0

r2=1.37013943  
r3=0.99366816  
r4=0.99366816  
a3=105.32548592  
a4=105.32548592  
d4=119.02434528

--- Geometry Optimization ---

1\1\GINC-PAULING\POpt\RM062X\6-311++G(3df,2p)\F1H2O1(1+)\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\F,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\r2=1.37013943\r3=0.99366816\r4=0.99366816\a3=105.32548592\a4=105.32548592\d4=119.02434528\Version=IA64L-G09RevA.02\State=1-A\HF=-175.7597544\RMSD=1.468e-09\RMSF=7.009e-05\Dipole=0.3944275,-0.6699304,-1.3333429\Quadrupole=0.0273944,-1.0859972,1.0586027,1.0033001,-0.7913212,1.3440498\PG=CS [SG(F1O1),X(H2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\F1H2O1(1+)\ROSMUS\20-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\1,1\O\F,1,1.37013943\H,1,0.993668158,2,105.32548592\H,1,0.993668158,2,105.32548592,3,119.02434528,0\Version=IA64L-G09RevA.02\State=1-A\HF=-175.0522678\RMSD=5.986e-09\Dipole=0.4059397,-0.6894838,-1.3296538\Quadrupole=0.07808,-1.0394586,0.9613787,1.0070371,-0.8007402,1.3600477\PG=CS [SG(F1O1),X(H2)]\@

HF=-175.7597544

Sum of electronic and zero-point Energies= -175.732341  
Sum of electronic and thermal Energies= -175.729440  
Sum of electronic and thermal Enthalpies= -175.728496  
Sum of electronic and thermal Free Energies= -175.754610  
NImag=0

Ge1H5O1(1+)

-----  
1,1  
O

Ge,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.99188206  
r3=0.96699328  
r4=0.96693298  
a3=123.61008966  
a4=123.07383588  
d4=157.0741846  
r5=1.52378028  
r6=1.52276267  
r7=1.52270339  
a5=101.02296737  
a6=97.12123766  
a7=97.86880763  
d5=85.55903022  
d6=-34.44163523  
d7=205.67358455

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\Ge1H5O1(1+)\ROSMUS\26-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Ge,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\H,2,r7,1,a7,4,d7,0\r2=1.99188206\r3=0.96699328\r4=0.96693298\a3=123.61008966  
\a4=123.07383588\d4=157.0741846\r5=1.52378028\r6=1.52276267\r7=1.52270339\a5=101.02296737  
\a6=97.12123766\a7=97.86880763\d5=85.55903022\d6=-34.44163523\d7=205.67358455\\Version=IA64L-G09RevA.02\State=1-A\HF=-2154.9237677  
\RMSD=5.947e-09\RMSF=3.055e-05\Dipole=0.0424145,-0.2132374,-1.3117168\Quadrupole=-1.9085001,-4.3454886,6.2539887,0.5242809,-0.2474421,1.1308218\PG=C01 [X(Ge1H5O1)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Ge1H5O1(1+)\ROSMUS\26-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\1,1\O\Ge,1,1.9918820582\H,1,0.9669932831,2,123.61008966\H,1,0.966932975,2,123.07383588,3,157.0741846,0\H,2,1.5237802842,1,101.02296737,4,85.55903022,0\H,2,1.5227626724,1,97.12123766,4,-34.44163523,0\H,2,1.5227033923,1,97.86880763,4,205.67358455,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-2152.975514\RMSD=5.863e-09\Dipole=0.044638,-0.2226316,-1.3080241\Quadrupole=-1.9349464,-4.3628528,6.2977991,0.520801,-0.2543646,1.1578185\PG=C01 [X(Ge1H5O1)]\@

HF=-2154.9237677

Sum of electronic and zero-point Energies= -2154.875106  
Sum of electronic and thermal Energies= -2154.870222  
Sum of electronic and thermal Enthalpies= -2154.869278  
Sum of electronic and thermal Free Energies= -2154.901868  
NImag=0

H4N1O1(1+)

-----  
1,1  
O  
N,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0

r2=1.45092648  
r4=0.97655328  
r5=1.01994835  
a4=108.99663793  
a5=102.89037905  
d4=129.89519261  
d5=218.46444969  
r6=1.02039888  
a6=106.17399642  
d6=102.74171566  
r3=0.97758647  
a3=117.34712905

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H4N1O1(1+)\ROSMUS\20-Jul-2012\1\#\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\N,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d6,0\r2=1.45092648\r4=0.97655328\r5=1.01994835\ a4=108.99663793\ a5=102.89037905\ d4=129.89519261\ d5=218.46444969\r6=1.02039888\ a6=106.17399642\ d6=102.74171566\r3=0.97758647\ a3=117.34712905\ \Version=IA64L-G09RevA.02\State=1-A\HF=-131.9913926\RMSD=2.449e-09\RMSF=4.222e-05\Dipole=0.7195773,-0.1989597,-0.7199671\Quadrupole=-0.7745952,-1.0374881,1.8120834,0.240388,0.8030069,2.1303336\PG=C01 [X(H4N1O1)]\@\

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H4N1O1(1+)\ROSMUS\20-Jul-2012\0\#\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\title\1,1\O\N,1,1.45092648\H,1,0.9775864676,2,117.34712905\H,1,0.9765532766,2,108.99663793,3,129.89519261,0\H,2,1.0199483467,1,102.89037905,4,218.464

44969,0\H,2,1.0203988839,1,106.17399642,4,102.74171566,0\\Version=IA64L-G09RevA.02\State=1-A\HF=-131.3436698\RMSD=3.325e-09\Dipole=0.7505369,-0.1957322,-0.6665869\Quadrupole=-0.7498117,-0.9985451,1.7483568,0.2400954,0.8315148,2.1690542\PG=C01 [X(H4N1O1)]\@

HF=-131.9913926

Sum of electronic and zero-point Energies= -131.938172  
Sum of electronic and thermal Energies= -131.934794  
Sum of electronic and thermal Enthalpies= -131.933849  
Sum of electronic and thermal Free Energies= -131.960968  
NImag=0

H3O2(1+)

-----  
1,1  
O  
O,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0

r2=1.42040886  
r3=0.98456938  
r4=0.98457804  
r5=0.97863382  
a3=106.27758798  
a4=106.27785925  
a5=101.26948883  
d4=118.43203399  
d5=239.21612234

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H3O2(1+)\ROSMUS\20-Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\\title\\1,1\O\O,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\\r2=1.42040886  
\r3=0.98456938\r4=0.98457804\r5=0.97863382\a3=106.27758798\a4=106.27785925\a5  
=101.26948883\d4=118.43203399\d5=239.21612234\\Version=IA64L-G09RevA.02\State=1-A\HF=-151.8092195\RMSD=9.558e-09\RMSF=5.298e-05\Dipole=0.0352073,-0.0591143,-0.9065354\Quadrupole=-0.5126787,-0.5184666,1.0311453,0.0053646,-1.7061921,2.8640253\PG=C01 [X(H3O2)]\@

--- NBO Single Point ---

1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H3O2(1+)\ROSMUS\20-Jul-2012\0\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck  
guess=read\\title\\1,1\O\O,1,1.4204088562\H,1,0.9845693813,2,106.27758798\H,1,0.984

5780378,2,106.27785925,3,118.43203399,0\H,2,0.9786338166,1,101.26948883,4,239.21  
612234,0\Version=IA64L-G09RevA.02\State=1-A\HF=-151.1236067\RMSD=2.314e-  
09\Dipole=0.0271222,-0.0455435,-0.8466211\Quadrupole=-0.464206,-  
0.4667554,0.9309615,0.0023745,-1.7446644,2.9286056\PG=C01 [X(H3O2)]\@

HF=-151.8092195

Sum of electronic and zero-point Energies= -151.769057  
Sum of electronic and thermal Energies= -151.765851  
Sum of electronic and thermal Enthalpies= -151.764907  
Sum of electronic and thermal Free Energies= -151.791601  
NImag=0

H5O1Si1(1+)

-----  
1,1  
O  
Si,1,r2  
H,1,r3,2,a3  
H,1,r4,2,a4,3,d4,0  
H,2,r5,1,a5,4,d5,0  
H,2,r6,1,a6,4,d6,0  
H,2,r7,1,a7,4,d7,0

r2=1.83047228  
r3=0.96934336  
r4=0.96934727  
a3=123.38820166  
a4=123.36105988  
d4=161.48620102  
r5=1.46016909  
r6=1.45967087  
r7=1.45968462  
a5=103.49022422  
a6=99.50468978  
a7=99.50773661  
d5=80.62460928  
d6=-39.34064039  
d7=200.59906449

--- Geometry Optimization ---

1\1\GINC-PAULING\FOpt\RM062X\6-311++G(3df,2p)\H5O1Si1(1+)\ROSMUS\26-  
Jul-2012\1\#p m062x 6-311++G(3df,2p) opt=(z-matrix,noeigen) optcyc=100  
freq\title\1,1\O\Si,1,r2\H,1,r3,2,a3\H,1,r4,2,a4,3,d4,0\H,2,r5,1,a5,4,d5,0\H,2,r6,1,a6,4,d  
6,0\H,2,r7,1,a7,4,d7,0\r2=1.83047228\r3=0.96934336\r4=0.96934727\a3=123.38820166

```

\a4=123.36105988\d4=161.48620102\r5=1.46016909\r6=1.45967087\r7=1.45968462\a5
=103.49022422\a6=99.50468978\a7=99.50773661\d5=80.62460928\d6=-
39.34064039\d7=200.59906449\\Version=IA64L-G09RevA.02\State=1-A\HF=-
367.4321545\RMSD=5.123e-09\RMSF=4.743e-05\Dipole=0.0279051,-0.171331,-
1.0624241\Quadrupole=-1.2500836,-3.8556107,5.1056943,0.4364164,-
0.1346739,0.8293097\PG=C01 [X(H5O1Si1)]\ \@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\H5O1Si1(1+)\ROSMUS\26-Jul-2012\0\#p
hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck
guess=read\\title\\1,1\O\Si,1,1.8304722843\H,1,0.9693433639,2,123.38820166\H,1,0.96
9347268,2,123.36105988,3,161.48620102,0\H,2,1.4601690859,1,103.49022422,4,80.624
60928,0\H,2,1.4596708727,1,99.50468978,4,-
39.34064039,0\H,2,1.4596846211,1,99.50773661,4,200.59906449,0\\Version=IA64L-
G09RevA.02\State=1-A\HF=-366.521125\RMSD=2.965e-09\Dipole=0.0294381,-
0.1807764,-1.0862635\Quadrupole=-1.2966938,-3.8930694,5.1897633,0.4349082,-
0.1386007,0.8532199\PG=C01 [X(H5O1Si1)]\ \@

```

HF=-367.4321545

```

Sum of electronic and zero-point Energies=      -367.381447
Sum of electronic and thermal Energies=         -367.376873
Sum of electronic and thermal Enthalpies=       -367.375929
Sum of electronic and thermal Free Energies=    -367.406702
NImag=0

```