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Excess Valency as an Intrinsic Scale of Lewis Basicity

Joseph J. Rosmus

EXCESS VALENCY AS AN INTRINSIC SCALE OF LEWIS BASICITY

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By

Joseph J. Rosmus

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Approved November 20, 2013

_____	_____
Jeffrey D. Evanseck Professor of Chemistry and Biochemistry Thesis Director (Committee Chair)	Ellen S. Gawalt Associate Professor of Chemistry and Biochemistry (Committee Member)
_____	_____
Douglas J. Fox Director, Gaussian Inc. (External Reader)	Jeffry D. Madura Lambert F. Minucci Endowed Chair in Engineering and Computational Sciences Professor of Chemistry and Biochemistry (Committee Member)
_____	_____
Philip Reeder Dean, Bayer School of Natural and Environmental Science Professor	Ralph A. Wheeler Chair, Department of Chemistry and Biochemistry Professor of Chemistry and Biochemistry

ABSTRACT

EXCESS VALENCY AS AN INTRINSIC

SCALE OF LEWIS BASICITY

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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.[1,2] 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.[3-12] 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.[13,14]

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.[2] Some of these factors are orbital and steric interactions.[15] It is well known that using the adduct's bond strength can lead to confusing results. For instance, when comparing two acids, such as BF_3 and BH_3, it is found that BH_3 bonds more strongly with thioethers, while BF_3 bonds more strongly with ethers.[16] Another instance where the use of thermodynamic data yields unexpected results is the anomalous ordering of methylated amine basicities.[17] As methyl groups are substituted in for hydrogens of ammonia, the basicities increase. However, the last substitution, trimethylamine, has a marked decrease in basicity.[17] A number of explanations have been proposed to explain the pattern of basicity in methylated amines including solvent effects,[18-21] sterics contributions from the methyl groups,[17,22] and inductive effects.[17-19,22-25]

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.[26] 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."[2] Laurence and Gal have summarized the data for four methods of defining Lewis base strength.[26,27] The first class is the *donor number* method of Ollofson.[28-40] In this method, the strength of the adduct bond formed between the base and $SbCl_5$ in 1,2-dicloromethane is determined. The affinity of the base for $SbCl_5$ (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 $SbCl_5$ affinity scale but differs in that it is a BF_3 affinity scale. The $SbCl_5$ and BF_3 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.

$$(Donor\ Number) = -4.83 + 1.09(BF_3\ affinity) \qquad \text{Equation 1}$$

The advantage in using the BF_3 affinity is that there is a larger number of bases that have been studied using the BF_3 affinity. However, these two methods do not always align. For example, the affinity of pyridine to $SbCl_5$ is stronger than that of triethylamine to $SbCl_5$, while the opposite is found for BF_3 affinity.[20,41,42]

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.[19,26,27,43] The equilibrium constant K_c is determined from the O-H stretching frequency of the hydrogen-bond donor.[19,26,27,43]

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.

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

A double-scale approach has been determined by Drago and Wayland that predicts the enthalpy of Lewis adduct formation using Equation 2.[6] 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, ΔH, 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.[6] 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.[6] 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.[6,17,22]

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.[44] 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.[45]

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 trisubstitued 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[46,47] and covalent radii[48] 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[49] 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)[50] 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

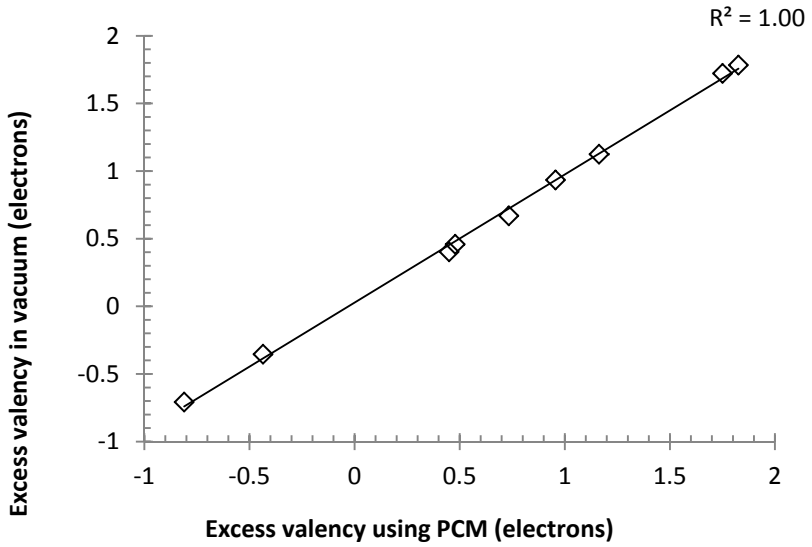

Figure 1. Comparison excess valency of tri-substituted amines for vacuum and implicitly solvated calculations

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.[44,51,52] The systems evaluated include $BH_3NX_nH_{(3-n)}$ and $NX_nH_{(3-n)}$ (X=CH_3, SiH_3, GeH_3, OH, SH, SeH, 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_2, SXH, SX_2, PXH_2, PX_2H, PX_3 (X=CH_3, SiH_3, GeH_3, 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_3H_2, $\bar{\chi}_{sub}$=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.[53-61] These geometries were then validated as minima and thermodynamic properties were calculated

using a frequency analysis.[62] All calculated molecular energies were corrected for basis set superposition error using the counterpoise method of Boys and Bernardi[63] as well as the PCM model[64,65] 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[66-69] was performed using the NBO 5.9 program,[45] embedded within the Gaussian 09 suite. NBO transforms the non-orthogonal atomic orbitals from the HF wave function into orthonormal natural atomic orbitals

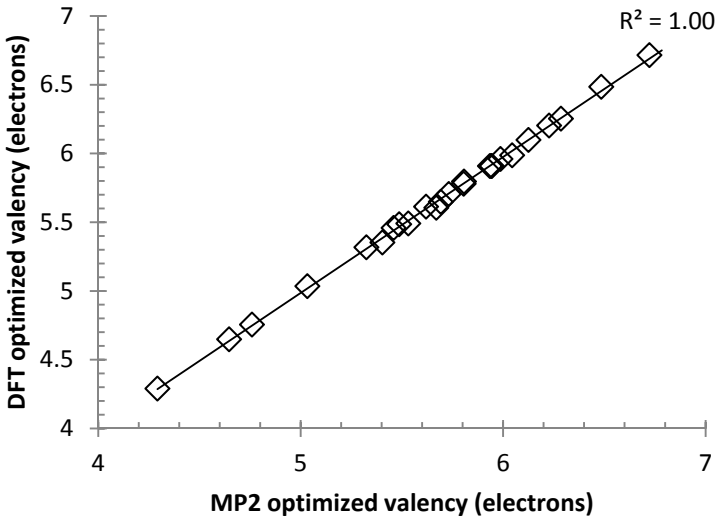

Figure 2. Comparison excess valency of tri-substituted amines DFT and MP2 calculations.

(NAO),[70] natural hybrid orbitals (NHO),[71] natural bond orbitals (NBO)[66] and natural localized molecular orbitals (NLMO).[72] 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.[73] 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

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

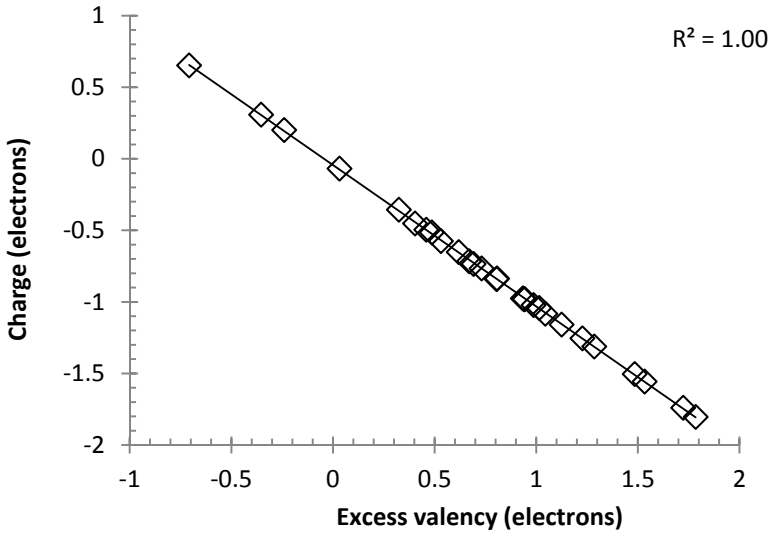

Figure 3. Comparison for excess valency of substituted amines with the charge

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.

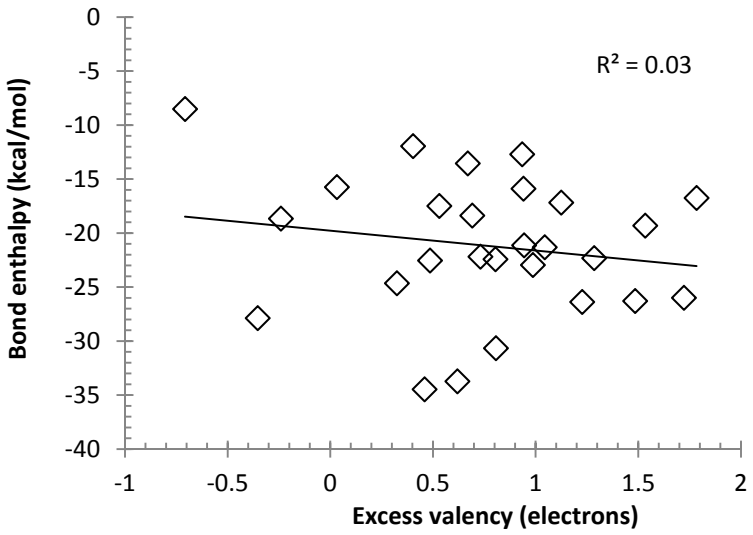

Figure 4. Bond enthalpy of $BH_3NH_{(3-n)}X_n$ compared with the excess valency of the isolated base.

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.

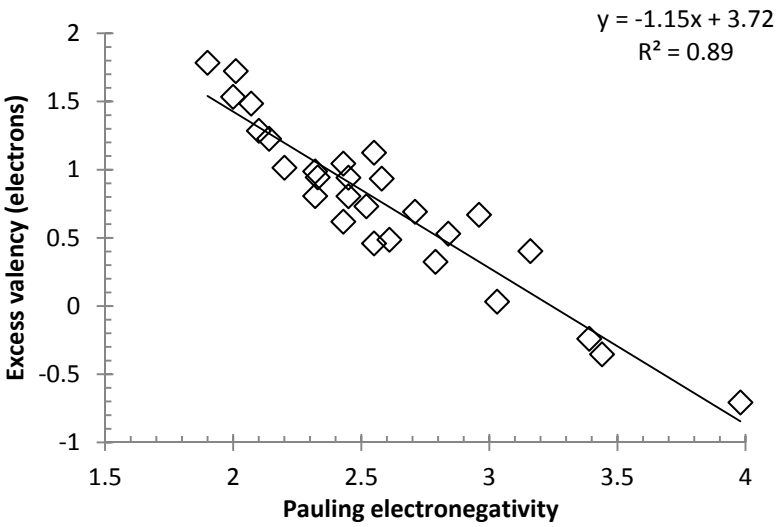

Figure 5. Correlation for excess valency of the nitrogen of 28 isolated amines with average Pauling Electronegativity of the atom bound to the nitrogen

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.

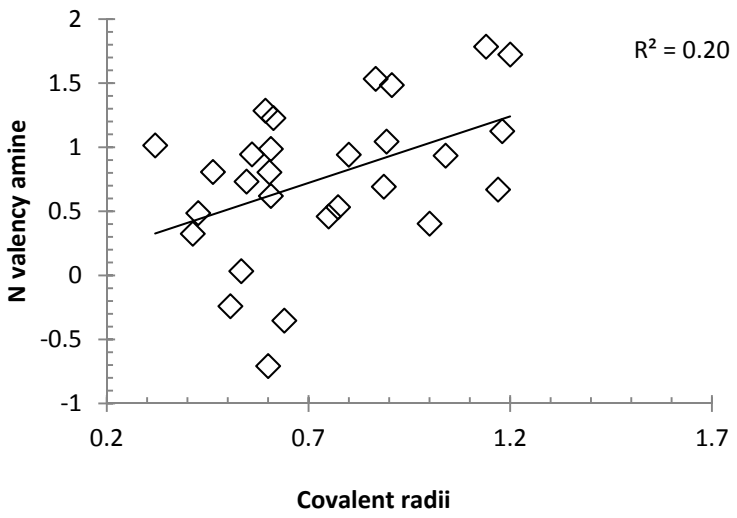

Figure 6. Correlation between the excess valency of the nitrogen for 28 isolated amines and the average radii of the atoms bound to the nitrogen.

When second period amines ($NH_{3-n}(CH_3)_n$, $NH_{3-n}(OH)_n$, $NH_{3-n}F_n$) 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 ($NH_{3-n}(SiH_3)_n$, $NH_{3-n}(SH)_n$, $NH_{3-n}Cl_n$), 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 ($NH_{3-n}(GeH_3)_n$, $NH_{3-n}(SeH)_n$, $NH_{3-n}Br_n$) 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 ($NH_{3-n}(CH_3)_n$, $NH_{3-n}(SiH_3)_n$, $NH_{3-n}(GeH_3)_n$)(R^2=0.97), group 16 ($NH_{3-n}(OH)_n$, NH_{3-}

$_n(SH)_n$, $NH_{3-n}(SeH)_n$) (R^2=0.88), and group 17 ($NH_{3-n}F_n$, $NH_{3-n}Cl_n$, $NH_{3-n}Br_n$) (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.

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

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.

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

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.

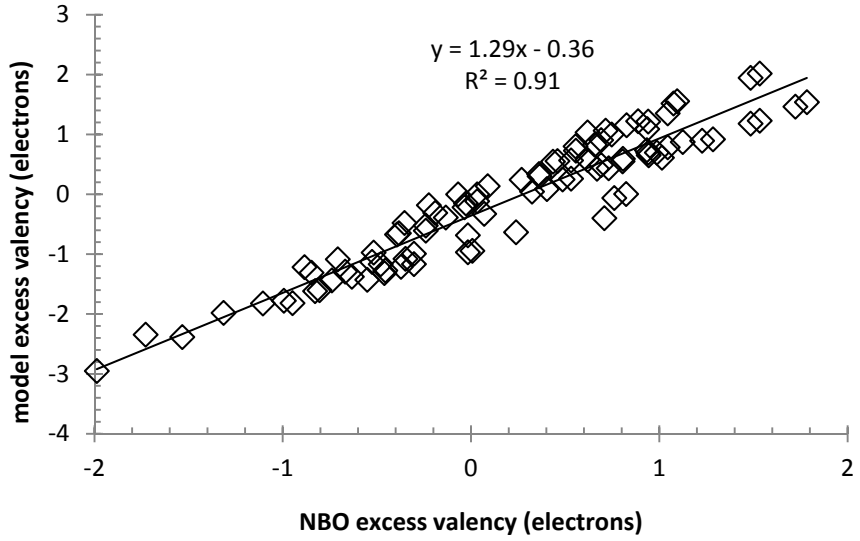

Figure 7. Comparison between the NBO calculated excess valency and that calculated using Equation 4

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 I2 halogen bond for primary amines increases as the carbon chain increase in size from 20.1 for ammonia to 35.1 for n-butylamine.[26,74] 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_2 (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_3, p-Cl, p-F, p-H, p-OH, m-Cl, p-CH_2CH_3, p-$CH_2CH_2CH_3$, p-OCH_3, and p-OCH_2CH_3). 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

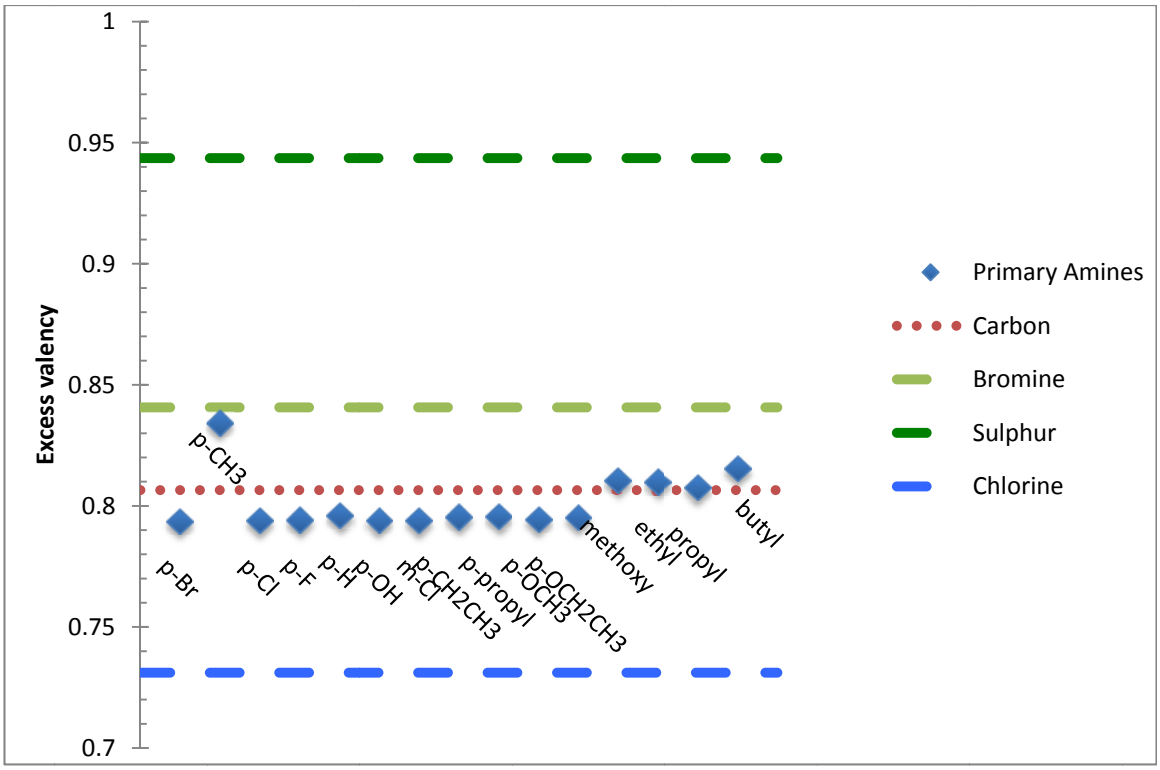

Figure 8. Investigation of primary amines where the atoms directly bound to the nitrogen are held constant and the variation is seen beyond the carbon. Lines shown represent the bases investigated in Chapter 3 with a valency closest to those investigated herein.

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 NH_2CN and $NH_2C_6H_4Br$, respectively. The variation in excess valency when the bound atoms were varied resulted in a maximum of 1.784 for $N(SiH_3)_3$ and a minimum of -0.707 for 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.[75]

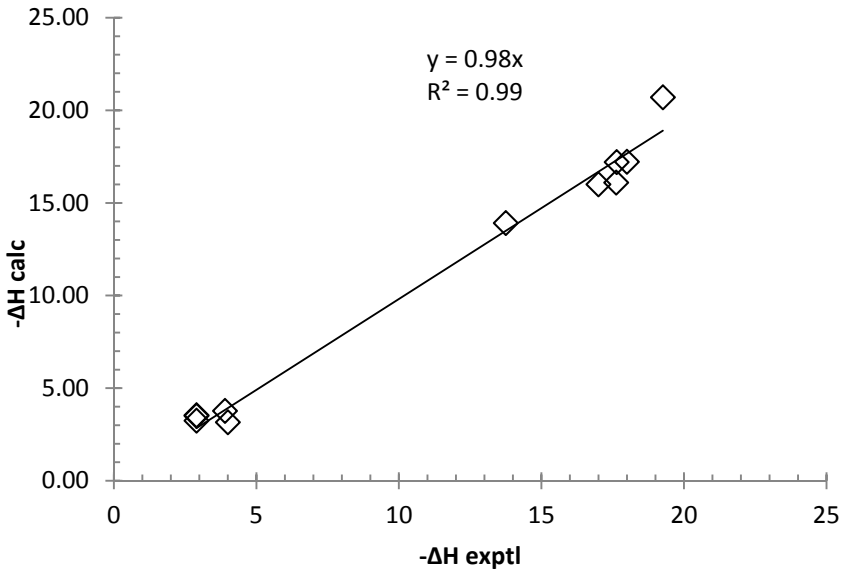

Figure 9. A straight line is realized when the bond enthalpy is calculated by equation 5 is plotted against the bond enthalpy from experiment. The lower cluster belongs to the bases complexed to I_2 and the higher to those complexed with $B(CH_3)_3$

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.[6] 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,[6] 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

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

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 –ΔH *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	-ΔH *exptl* (kcal/mol)	-ΔH *calc* (kcal/mol)
$B(CH_3)_3$	NH_3	1.34	1.37	13.7[22]	13.8
$B(CH_3)_3$	NH_2CH_3	1.19	1.11	17.6[22]	17.7
$B(CH_3)_3$	$NH(CH_3)_2$	0.94	0.87	19.3[22]	20.7*
$B(CH_3)_3$	$N(CH_3)_3$	0.59	0.67	17.6[22]	23.8*
$B(CH_3)_3$	$NH_2(C_2H_5)$	1.26	1.11	18.0[22]	18.1
$B(CH_3)_3$	NC_5H_5	0.88	0.66	17.0[76]	17.3
$(CH_3)_3COH$	$O(CH_2)_4$	0.61	0.81	2.9[77]	3.5
$(CH_3)_3COH$	NC_5H_5	0.88	0.66	4.0[77]	3.2
$(CH_3)_3COH$	$CO(CH_3)_2$	0.706	0.84	2.9[77]	3.2
$(CH_3)_3COH$	$CH_3COOC_2H_5$	0.639	0.88	2.9[77]	3.5
$(CH_3)_3COH$	$HCON(CH_3)_3$	0.97	0.93	3.9[77]	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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NImag=0

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--- NBO Single Point ---
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NImag=0

B1Br2H4N1

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r8=1.01840998
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Sum of electronic and thermal Enthalpies= -5230.200486
Sum of electronic and thermal Free Energies= -5230.237981
NImag=0

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

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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=110.19931492\\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,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\\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=(nboread,savenbos) guess=read geom=allcheck\\title\\0,1\B\N,1,1.6344695953\H,1,1.2065742322,2,105.3402816\H,1,1.2064287194,2,105.05457064,3,120.09490643,0\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,2,1.0951719958,1,114.8201245,4,59.0182916,0\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,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,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=(nboread,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,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,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\r
3=1.20732792\r4=1.20739584\r5=1.2072536\r6=1.47515235\r7=1.47528871\r8=1.47530
987\r9=1.0920814\r10=1.08683481\r11=1.08683652\r12=1.09208016\r13=1.08703978\r
14=1.086927\r15=1.09202397\r16=1.08707543\r17=1.08687285\a3=105.3247753\a4=10
5.34844742\a5=105.31310193\a6=109.59737583\a7=109.56857584\a8=109.53163401\a
9=110.24497557\a10=108.60055327\a11=108.59430968\a12=110.26567162\a13=108.62
511588\a14=108.53894346\a15=110.28115543\a16=108.55294572\a17=108.58001841\d
4=120.12159195\d5=240.11616671\d6=179.23401111\d7=59.20423756\d8=299.219344
88\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)]\\@
--- NBO Single Point ---
1\1\GINC-MH325M16MH\SP\RHF\CC-pVQZ\C3H12B1N1\ROSMUSJ\18-Jun-
2012\0\\#p hf/cc-pvqz scf=verytight pop=(nboread,savenbos) guess=read
geom=allcheck\\title\\0,1\B\N,1,1.6392227445\H,1,1.2073279236,2,105.3247753\H,1,1.2
073958428,2,105.34844742,3,120.12159195,0\H,1,1.2072535978,2,105.31310193,3,240.
11616671,0\C,2,1.4751523502,1,109.59737583,3,179.23401111,0\C,2,1.4752887086,1,1
09.56857584,3,59.20423756,0\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,8,1.0920239687,2,110.2811554
3,1,179.5614837,0\H,8,1.0870754297,2,108.55294572,1,58.73400542,0\H,8,1.08687284
82,2,108.58001841,1,300.39139057,0\\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)]\\@

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=1.44901212\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\\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,2,1.103386006,1,112.10391305,4,61.52188044,0\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

B1Cl1H5N1

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)\B1Cl1H5N1\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=100.44810494\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\\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(B1Cl1H5N1)]\\@
--- NBO Single Point ---
1\1\GINC-MH325M14MH\SP\RHF\CC-pVQZ\B1Cl1H5N1\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\\Versio
n=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(B1Cl1H5N1)]\\@

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\r
4=1.01574087\a3=104.98426144\a4=104.98426144\d4=111.80333713\\Version=EM64
M-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=(nboread,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=101.60696092\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\\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,1,1.1976068051,2,101.59748983,3,240.04731396,0\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=EM64M-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,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\\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,1,1.1980668508,2,105.91851696,3,118.24854785,0\H,1,1.1984337894,2,105.84078783,3,242.18407076,0\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\\Version=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,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\\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 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=(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\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\\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,1,1.6501082651\H,1,1.2036415188,2,106.93796891\H,1,1.2062432107,2,104.97877331,3,121.04175256,0\H,1,1.2108889017,2,104.84199247,3,239.55911136,0\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,6,1.5286188858,2,106.29781452,1,46.65642665,0\H,6,1.5313351607,2,105.36621066,1,284.95575126,0\\Version=EM64M-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\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\\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\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\\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=(nboread,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=179.89909983\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\\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,2,1.54627202,1,110.80802925,4,60.27341432,0\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\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\\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)]\\@
--- 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,2,1.5456368804,1,110.5812208,4,119.49234429,0\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\\Version=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=1.01825194\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\\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=(nboread,savenbos) guess=read geom=allcheck\\title\\0,1\B\N,1,1.6242753945\H,1,1.210413464,2,101.23995432\H,1,1.1998346802,2,105.4776888,3,118.82623222,0\H,1,1.2000079301,2,105.43247159,3,241.34598169,0\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,6,0.9641319981,2,107.55892295,1,180.97826466,0\\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,2,0.9586809457,1,103.47281683,4,235.70451328,0\\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,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\\Version=EM64M-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,1,1.1967924307,2,104.81450684,3,238.9230429,0\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)]\\@
--- 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=103.53619422\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,2,0.9622674271,1,103.52246625,4,206.08035498,0\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=1.01502585\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\\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=1.855743 12\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,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\\Version=EM64M-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,1,1.203653072,2,104.09708273,3,119.70596777,0\H,1,1.2029117951,2,104.53576123,3,239.83231739,0\Se,2,1.8893015074,1,107.6645979,3,185.21596456,0\Se,2,1.8895588797,1,107.46893972,3,57.58691503,0\H,2,1.0154896672,1,106.93896212,3,301.46863338,0\H,6,1.4734322419,2,94.97070264,1,183.26046317,0\H,7,1.4733139569,2,95.01763466,1,177.1586216,0\\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=1.47803171\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,1,1.8524007976,2,98.62403914,3,120.,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,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\\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=(nboread,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,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=107.668696223\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\\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,1,1.2091416632,2,104.24495926,3,241.18987833,0\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,6,1.4663737687,2,109.14774163,1,44.1044687,0\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,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\\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=(nboread,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,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\\Version=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,-
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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,-
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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,-
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.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,-
0.00178470,0.00169364,0.00023994,0.07643955,0.16762827,-0.01653911,-0.02978211,-
0.04477020,-0.01243439,-0.02234338,-
0.02215581,0.00285533,0.00537772,0.00532619,0.02352110,0.04229428,0.05900350,-
0.07829029,0.06590015,-0.02039199,0.00316720,-0.00073357,-0.00374372,-
0.01017693,0.01864059,-0.00608094,0.00746305,-
0.00848192,0.00333488,0.07974430,0.06496701,-0.15562281,0.03311922,-
0.00028386,0.00503776,0.00504142,0.00196737,0.00144348,-0.00018185,0.00818076,-
0.01609415,0.00530371,-0.07572538,0.16889655,-0.01741098,0.02904667,-
0.04467154,-0.01316903,0.02199341,-0.02217017,0.00296014,-
0.00554803,0.00533776,0.00322651,-0.00520906,0.00533586,0.02477752,-
0.04135188,0.05892244,-0.00120355,-0.00061562,0.02426606,-0.13683464,-

0.03715415,0.01823046,0.00049759,0.00045490,-0.00427265,-0.00244306,-
0.00262389,-0.00345357,-0.00195731,0.00260492,-
0.00404591,0.34862964,0.00048365,0.00452679,0.01274223,-0.03689272,-
0.07303462,0.00798348,0.00082785,-0.00129202,-0.00287445,-0.00196489,-
0.00471507,-0.00180947,-0.00042156,-0.00181851,-0.00147421,-
0.02159921,0.37033351,0.01810284,0.01173012,-0.00395923,0.02650971,0.01250082,-
0.05262995,-0.00375966,-0.00193051,-0.00402361,-0.00392929,-
0.00309800,0.00151096,-0.00065487,-0.00216436,-0.00042995,0.01891673,-
0.00212610,0.33768429,0.00313414,-0.00301247,-0.00109571,-0.05694631,-
0.00922166,-0.00219953,-0.00280562,0.00091160,0.00074661,-
0.00139325,0.00026254,-0.00035272,-0.00217585,0.00179672,0.00015858,0.00003574,-
0.02528967,-0.00481480,0.38409553,-0.00190890,0.00013889,-0.02742530,-
0.00899214,-0.15322793,-0.01966976,-0.00212791,-
0.00099041,0.00423790,0.00064014,0.00059446,0.00514012,0.00246302,-
0.00502175,0.00389322,-0.02663356,-
0.01539149,0.00207094,0.00124390,0.33563614,0.00112063,-0.02157531,-0.00389964,-
0.00240943,-0.02914869,-0.05252246,-0.00155404,0.00165160,-
0.00044640,0.00021331,0.00424162,-0.00402530,-0.00073815,0.00499902,0.00152475,-
0.00387544,0.00429404,0.01175725,-0.01152648,-
0.01537784,0.33732951,0.00303480,0.00199317,-0.02318707,-0.12108618,0.04587484,-
0.01600143,-0.00615807,-0.00019155,0.00328976,-
0.00090515,0.00102219,0.00330325,-0.00030219,-0.00128950,0.00462901,-
0.03401160,0.00559062,-
0.00172475,0.01093360,0.02037066,0.00416990,0.34589418,0.00305438,0.00031533,0.
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0.00198798,-0.00286181,-0.00276323,-0.00090855,-0.00050156,-
0.00225915,0.00694163,0.01862299,-0.00550175,0.01902998,-
0.02630471,0.00320318,0.02028544,0.37316393,-0.01922104,0.00978533,-0.00396478,-
0.02404563,0.01666692,-0.05262842,0.00464561,-
0.00184833,0.00152094,0.00219728,0.00051423,-0.00042826,0.00356036,-0.00230936,-
0.00403113,0.00064504,-0.00519443,0.01177814,0.00563342,0.00129445,0.01181380,-
0.00756748,0.01761696,0.33774111,-0.00303155,-0.00088600,-0.00354147,-
0.00551374,-0.00019998,0.01795356,0.00030625,-
0.00011658,0.00188364,0.00077470,0.00066196,0.00005622,0.00041905,-
0.00044283,0.00050122,-0.03546575,0.00554637,0.01736161,-
0.00022453,0.00382692,0.00004565,0.00264321,-0.00179563,0.00016847,0.03237440,-
0.00168113,-0.00064137,-0.00147198,-0.00426741,0.00493434,0.00734463,-
0.00003388,0.00035754,0.00083573,0.00054945,0.00100262,0.00002366,0.00005724,0.
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0.00127020,0.00018428,-0.00265074,0.00077972,-0.00502319,0.03386891,0.00098461,-
0.00040652,0.00019270,0.00483787,0.00049691,-0.00217495,0.00051169,0.00021800,-
0.00040084,0.00041097,0.00038428,-0.00006963,-0.00000252,0.00016128,-
0.00000877,0.02031425,-0.03075927,-0.17169712,0.00001462,-0.00208946,-
0.00250309,-0.00149070,0.00143024,-0.00239057,-
0.02635424,0.03436129,0.18409495,-0.00026880,0.00008722,-0.00225986,-
0.00292045,-0.01904617,0.00026147,0.00009381,-0.00009355,0.00026132,0.00011775,-

0.00012270,0.00041281,0.00042686,-0.00034773,0.00034600,-
0.03243807,0.01855707,0.00037508,-
0.00270857,0.00294251,0.00212421,0.00378542,0.00043013,0.00014671,0.00372893,0.
00230798,0.00063635,0.02844930,0.00006347,-0.00046397,-0.00201477,-0.00505574,-
0.00700249,0.00004635,-
0.00017564,0.00022766,0.00030240,0.00028634,0.00071372,0.00021371,-
0.00005151,0.00021850,0.00027755,0.01402710,-0.18635780,-0.01925047,-
0.00001870,0.00166101,0.00084412,0.00120377,-0.00355846,0.00068996,0.00074861,-
0.00162734,-0.00195441,-0.01239251,0.19930793,-0.00094709,-0.00081494,-
0.00111045,0.00108333,0.00369373,0.00365482,0.00047731,0.00036671,0.00036889,0.
00121985,0.00181147,-0.00041857,0.00033631,0.00049204,0.00023227,-0.00033447,-
0.02198024,-0.03355318,0.00086531,-0.00017277,-0.00182001,-
0.00008567,0.00046211,-0.00188600,0.00157614,-0.01433469,-0.00041716,-
0.00280583,0.02220256,0.02911881,-0.00007887,0.00051070,-0.00268013,-
0.01528837,0.00299529,-0.00459575,-0.00017353,-0.00011579,0.00024216,-
0.00025184,0.00011345,0.00046709,0.00023990,-0.00032673,0.00035761,-
0.10877286,0.04812429,-0.06618672,-0.00026724,0.00362408,0.00086012,0.00086779,-
0.00355690,0.00123312,0.00441964,0.00004075,0.00001799,0.00209039,0.00167235,-
0.00125359,0.11780604,-0.00003818,-0.00111194,-0.00097393,-
0.00637328,0.00578756,-0.00198611,-
0.00015934,0.00038028,0.00000479,0.00056525,0.00053792,0.00014435,-
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0.00034073,-0.00000703,-0.00062637,0.00171751,0.00058099,-0.04634048,-
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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,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\\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 ---
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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,2,1.3399078551,1,97.34401014,4,241.31912163,0\\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,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\\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\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\\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\S,2,1.7589870037,1,104.75852749,3,185.65030702,0\S,2,1.7687829231,1,110.75138257,3,63.01306941,0\S,2,1.7570648539,1,105.24853914,3,306.21767686,0\H,6,1.3433226489,2,95.45901676,1,187.19485192,0\H,7,1.3412304154,2,93.48216539,1,4

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,1,1.7375405077,2,108.51059986,3,117.83994713,0\\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,1,1.3509406581,2,102.01806214,3,105.27979459,0\\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\aH1=97.4404465\aH2=97.5205837\aH3=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,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=1.4790

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=179.99646965\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\\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\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\\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\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,1,1.3971920553,2,114.97022466,3,131.90876931,0\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,7,1.3891401522,5,121.54181114,1,-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,9,1.5133409082,7,123.35377764,8,180.03048217,0\H,14,1.0935152203,9,108.52946981,7,122.87487572,0\H,14,1.0934320705,9,108.54667194,7,-122.64869766,0\C,14,1.5232188179,9,115.3437217,7,0.1373714,0\H,17,1.0908171863,14,111.23326428,16,182.79388497,0\H,17,1.0907443496,14,111.26695491,16,62.41206181,0\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-methylanaline\\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-methylanaline\\0,1\N,0,0.0049738716,-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-Chloroanaline\\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-Chloroanaline\\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\Cl,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(C6H6Cl1N1)]\\@

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=1.0
8226435\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=120.5
5675163\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\\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,1,1.393
8700739,2,115.07781194,3,133.83260196,0\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,7,1.388314955
5,5,120.77522141,1,-
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,9,1.080680915
3,7,120.55675163,8,-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=1.39443165\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\\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,1,1.4029985969,2,114.05155922,3,129.90767278,0\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,7,1.3878482715,5,120.15475003,1,-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,9,1.3664220586,7,117.7258743,8,-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=(nboread) 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)\Cl1H1O1\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(Cl1H1O1)]\\@
--- 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,2,1.087685577,1,106.94346869,3,180.,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

Cl1H1O1

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)\Cl1H1O1\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(Cl1H1O1)]\\@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl1H1O1\ROSMUS\23-Jul-2012\0\\#p hf/cc-pvqz scf=verytight pop=(nboread) geom=allcheck guess=read\\title\\0,1\O\Cl,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(Cl1H1O1)]\\@

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=IA64L-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

0,1
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\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\\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\P\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,1,1.800207852\H,1,0.9602966103,2,107.799023\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=(calcall,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.,2,95.577,3,266.6448,0\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,1,1.6761360716\Cl,1,1.6761372576,2,112.22346452\\Version=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,3,1.47369 2814,1,95.68002165,2,275.18331414,0\\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\\#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\\#p 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,2,1.4734688393,1,108.88086973,4,125.96318543,0\H,2,1.4748700248,1,109.78559184,4,366.12135103,0\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\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\\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\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\\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\P\C,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

Cl1H2P1

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\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\\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\P\N,1,1.7036703901\H,1,1.4187659279,2,103.15501073\H,1,1.4115252869,2,98.78087673,3,95.05519339,0\H,2,1.0070101063,1,114.70516235,4,200.5055 1009,0\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,1,1.4131047791,2,93.57633853,3,93.74475721,0\H,2,1.4767595165,1,113.34377487,4,46.87086949,0\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\r4=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\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\\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\P\C,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=265.67464366\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\\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,1,1.4131780589,2,93.84070531,3,265.67464366,0\H,2,1.5414472562,1,108.89098624,4,76.8504384,0\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\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=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,1,1.4073427331,2,93.93254839,3,94.95730976,0\H,2,0.9588681775,1,111.75668656,4,203.23963646,0\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,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\\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,2,1.4659615259,1,92.12503384,4,204.81511908,0\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=107.13305937\a4=97.5801963\a5=99.37862637\a6=99.36108892\d4=259.7062433\d5=319.33828471\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,1,1.405791098,2,97.5801963,3,259.7062433,0\H,2,1.3394091997,1,99.37862637,4,319.33828471,0\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\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\\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\P\C,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 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)]\\@

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\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\\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,1,1.62
41571189,2,97.65172859,3,98.77260133,0\H,2,0.9599493911,1,112.42813757,4,197.526
35852,0\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=1.4
7090858\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\P\X,1,1.\Se,1,2.2615761992,2,114.06278331\Se,1,2.2615761992,2,114.06278331,3,120.,0\Se,1,2.2615761992,2,114.06278331,3,-120.,0\H,3,1.4709085762,1,96.77947541,2,180.,0\H,4,1.4709085762,1,96.77947541,2,180.,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\r4=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=102.14106407\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\\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,2,0.9786276572,1,102.00838039,4,220.04310367,0\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=127.14471136\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,1,0.973300169,2,116.57320251,3,186.32884986,0\H,2,1.3448137388,1,93.62775219,4,269.86971863,0\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,-0.1778782,0.049779\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,3,1.531315151,1,100.69624828,2,-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,4,1.4718976691,1,92.20985076,2,180.,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=93.46163183\a7=93.57263063\d4=181.83434307\d5=269.9233388\d6=270.97915707\d7=271.29456209\\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,1,1.7414372748,2,120.03108581,3,181.83434307,0\H,2,1.3444652069,1,93.55613284,4,269.9233388,0\H,3,1.3444456616,1,93.46163183,2,270.97915707,0\H,4,1.3445639989,1,93.57263063,3,271.29456209,0\\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 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=IA64L-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)\Cl1H1S1\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(Cl1H1S1)]\\@
--- NBO Single Point ---
1\1\GINC-PAULING\SP\RHF\CC-pVQZ\Cl1H1S1\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(Cl1H1S1)]\\@

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,1,1.339036792,2,94.38619911,3,252.01761264,0\H,2,1.5399475864,1,109.99829745,4,60.1509598,0\H,2,1.5400224919,1,110.03873802,4,-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,1,1.340069245,2,97.34109554,3,175.58481361,0\H,2,1.0101473649,1,111.06604867,4,241.41585064,0\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\S\Si,1,2.141380212\X,1,1.,2,110.65\H,1,1.3397948513,2,94.6020617,3,482.39621501,0\H,2,1.4740343293,1,111.19960438,4,60.45793114,0\H,2,1.4740857412,1,111.28041299,4,-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,1,0.9669932975,2,123.07383588,3,157.0741846,0\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,1,1.450926481\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,2,0.9786338166,1,101.26948883,4,239.21612234,0\\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,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\\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