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División de Ciencias Naturales y Exactas

A Theoretical Study of New Boron Ligands on the Activation of Small Molecules by a Diboron-Phosphine Ligand and on the Electronic Structure of Boron-Containing Heterocyclic Carbene (BNC) Gold Complexes.

Tesis

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Maestría en Ciencias Químicas

Presenta

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Abstract

A computational study was done for two different topics that are focused on the development of new boron ligands. The first topic corresponds to a study of the activation of small molecules by a bisborane-phosphine frustrated Lewis-pair (FLP), which contains two borane centers (9-Borabicyclo[3.3.1]nonane (9-BBN)) and one phosphine. The calculated reaction mechanism for these activations indicates that the second borane center confers a different reactivity to this FLP, as reflected in the reduction of H_2O to H_2, compared with the normal FLP that contains only one borane and a phosphine that only cleaves H-OH bond. Changing the 9-BBN boranes of this FLP, to a borane bearing cyclohexyls groups (Cy), increases the acidity of the boranes and, therefore, the FLP reactivity. This is because of the lowering of the overall total energy barriers and that this reaction with CO and H_2O does not generate the expected products. Theoretical calculations suggest that the migration of the cyclohexyls groups may be involved in producing these products, as the energy barrier for this migration is lower than the observed one with the previous FLP. The second topic is related to the study of the electronic properties and generation of the BNC gold(I) complexes, BNC-Au-L. These are accessed via the reaction of an azadiboriridine with a gold(I) complex and then, this reacts with an isocyanide to generate BNC-Au-L. Three different azadiboriridine derivatives were investigated to propose plausible reaction mechanisms. The mesityl azadiboriridine shows a reaction mechanism similar to that already reported for the tri(*tert*-butyl)azadiboriridine, but quite different to the reaction of (diisopropylamino)di(*tert*-butyl)azadiboriridine. The results show that the electron lone pair of the diisopropylamino group interacts with the adjacent borane which changes drastically the reaction. Moreover, the electronic structure of the BNC gold(I) complex was analyzed using Natural Bond Orbital (NBO), Intrinsic Bond Orbital (IBO) and Molecular Orbital theory. The findings indicate that this complex is more π–acceptor and σ–donor than the conventional CAAC and NHC gold(I) complexes. Furthermore, the reduction of the BNC gold(I) complex generates a 6π electron BNC ring, leading to a π–donating carbene species.

Resumen

En este trabajo, se realizó el estudio computacional de dos temas diferentes, los cuales están enfocados en el desarrollo de nuevos ligantes con boro. El primer tema corresponde al estudio de la activación de moléculas pequeñas por medio de un par frustrado de Lewis (FLP), una bisborano-fosfina, la cual contiene dos boranos (9-borabiciclo[3.3.1]nonano (9-BBN)) y una fosfina. Los mecanismos de reacción calculados para estas activaciones revelan que el segundo borano le confiere una reactividad diferente a este FLP, tal como se refleja en la reducción de H_2O a H_2, comparada con FLP normales que solo contienen un borano y una fosfina, que solo activan el enlace H-OH. El cambio de los boranos 9-BBN de este FLP a boranos que contienen ciclohexilos incrementa la acidez de estos nuevos boranos y, por lo tanto, la reactividad de este FLP. Esto es reflejado en la disminución de las barreras energéticas totales y en que su reacción con CO y H_2O no genera los productos esperados. Los cálculos sugieren que la migración de los ciclohexilos puede estar involucrada en la generación de estos productos, debido a que la barrera energética de esta migración es más rápida que la observada para el FLP previo. El segundo tema se relaciona con el estudio de las propiedades electrónicas y de la generación del complejo de oro(I). Estos complejos son generados mediante la reacción de un azadiboriridina con un complejo de oro(I) y después el complejo producido reacciona con el isocianuro para generar el complejo BNC-Au-L. Se investigaron tres derivados de azadiboriridina para estudiar sus mecanismos de reacción. El compuesto mesitil azadiboriridina tiene un mecanismo de reacción similar al ya reportado para la *tert*-butil azadiboriridina. Sin embargo, el mecanismo de reacción y el producto de reacción para la diisopropilamino azadiboriridina es diferente a los anteriores. Nuestros resultados muestran que el par de electrones del grupo diisopropiloamino interacciona con el borano adyacente y, por lo tanto, la reacción cambia totalmente. Además, la estructura electrónica de los complejos BNC oro(I) fue analizada mediante el uso de Orbitales Naturales de Enlace (NBO), Orbitales Intrínsecos de Enlace (IBO) y la teoría de Orbitales Moleculares. Los resultados indican que este complejo es más π−acceptor y σ−donador que los complejos convencionales de CAAC y NHC oro(I). También, la reducción del complejo BNC oro(I) genera un anillo BNC de 6 electrones π, el cual hace a este carbeno *p*-donador hacia el centro metálico.

Preface

In recent years, boron chemistry has widely increased due to its ability to do chemistry that transition metals do. Discovering chemistry that can replace transition metals for globally used reactions leads to a less harmful chemistry to the environment. Also, FLP chemistry has shown to activate small molecules of environmental importance. Thus, metal-free chemistry can be constituted by p-block elements, for example, phosphorus and boron. Therefore, its development leads to a greener chemistry.

On the other hand, the introduction of a boron atom to a heterocyclic carbene has shown to enhance its π–accepting and σ–donating properties compared to CAAC and NHC. Then, we can develop potential catalysts in which a high π–acceptor carbene is required for a specific reaction.

In this thesis, a theoretical study of two new boron-containing compounds is presented: One is related to the chemistry of Frustrated Lewis Pair and the other to heterocyclic carbenes. **Chapter 1** intends to review briefly the FLP and carbene chemistry with specific cases that are used to explain the results of this work. Then, **Chapter 2** compiles some background on theoretical and computational chemistry. In **Chapter 3**, the computational study of the new FLP, the bisborano-phosphine is presented. Therein, we discussed on the reaction mechanisms with small molecules, such as CO, H_2O, H_2, MeOH and others. After this, in **Chapter 4**, we studied the reaction mechanism for the formation of boron-containing carbenes BNC gold(I) complexes. Then, we analyzed the electronic structure of this new carbene by using the state-of-art computational techniques, namely IBO, NBO, ACID and NICS. All these calculations were based on the experimental work conducted at the University of Hiroshima. A detailed report about the synthesis and characterization of this chemistry is presented in the corresponding thesis of my coworkers Takumi Oishi and Yoshitaka Kimura.

Abbreviation Table

FLP	Frustrated Lewis Pair
NHC	N-Heterocyclic Carbene
CAAC	Cyclic(Alkyl)(Amino)Carbenes
BNC	Boron, Nitrogen-Containing Heterocyclic Carbene
NMR	Nuclear Magnetic Resonance
IBO	Intrinsic Bond Orbital
NBO	Natural Bond Orbital
NRT	Natural Resonance Theory
NICS	Nucleus-Independent Chemical Shifts
ACID	Anisotropy of the Induced Current Density
NOCV	Natural Orbital for Chemical Valence
DFT	Density Functional Theory
KS	Kohn-Sham
HF	Hartree-Fock
MO	Molecular Orbital
HOMO	Highest Occupied Molecular Orbital
LUMO	Lowest Unoccupied Molecular Orbital
CDA	Charge Decomposition Analysis
SCF	Self-Consistent Field
9-BBN	9-Borabicyclo[3.3.1]nonane
TMP	2,2,6,6-Tetramethylpiperidine
DMAP	4-Dimethylaminopyridine
DME	1,2-Dimethylether

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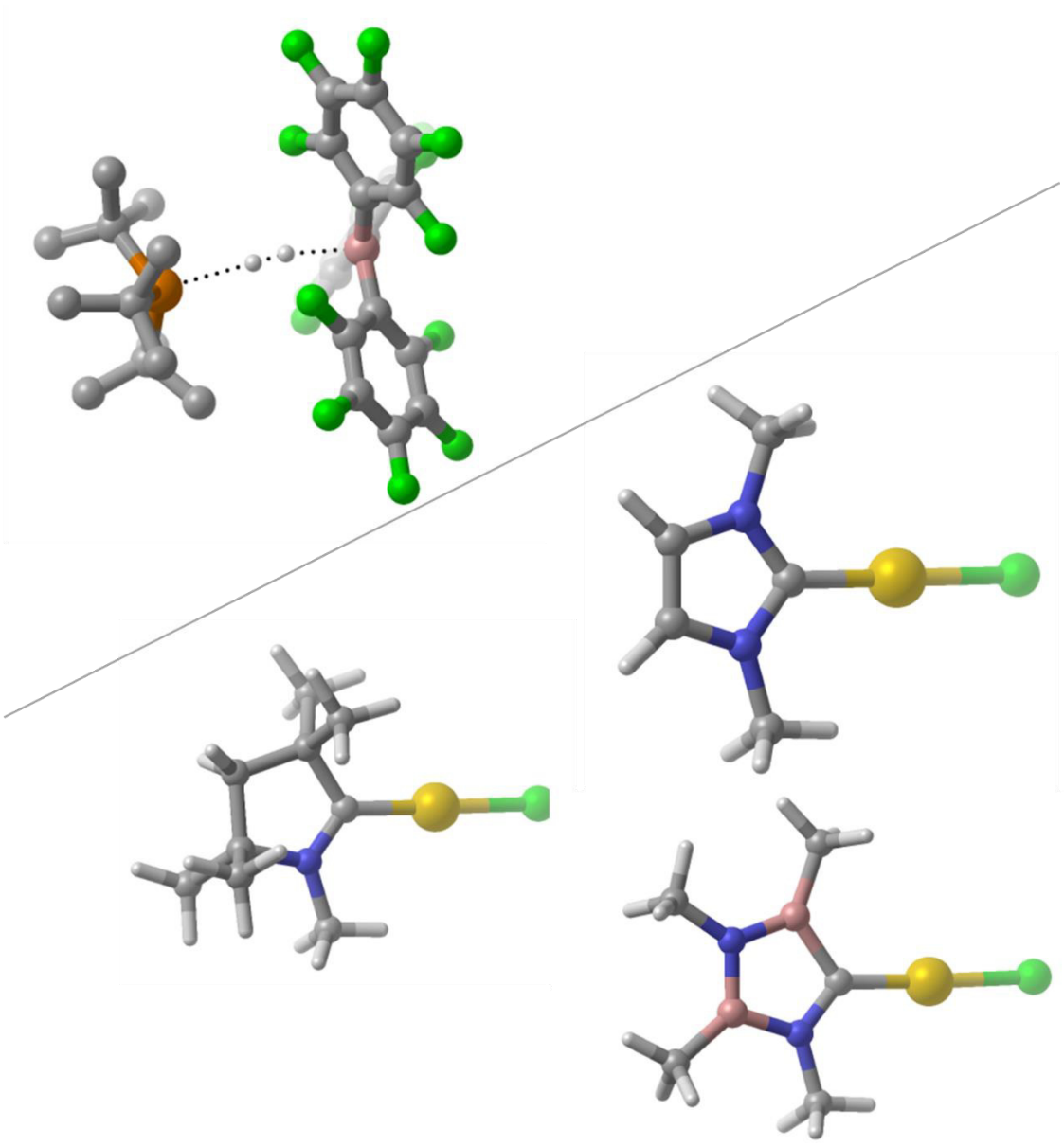
CHAPTER 1



In this chapter, two main topics are introduced: Frustrated Lewis Pairs (FLPs) and carbenes, both related to heterocyclic carbene chemistry. A brief history is given for each of these topics as well as its main chemistry and some specific topics that are relevant for our results.

In the Frustrated Lewis Pairs topic, we reviewed on the activation mechanism for the simple H–H molecule. We also investigated how the acidity and basicity of the donor and acceptor centers of FLPs affects the H–H activation. Then, we focus on the reactions of FLPs (P/B), containing phosphines and boranes combination, with small molecules such as CO_2, H_2O, and CO. These reactions are of great interest because the FLP bisborane-phosphine ligand, studied in posterior chapters, has a different reactivity. For example, it can reduce H_2O while previous FLPs containing phosphorus and boron are not capable of.

In the carbenes topic, we comment on the difference between Schrock and Fischer carbenes. From here, we specifically reviewed the heterocyclic carbenes, the N-Heterocyclic, cyclic alkyl(amino) carbenes (NHCs and CAACs) and the substituent ones with a p-block atom, such as boron or phosphorus. These are important because these are compared with the B-N-Heterocyclic carbenes (BNCs) in the results of the Thesis. After that, the π–accepting and σ–donating properties of the NHC–M–Cl (M = Cu, Ag, Au) complexes are described. Finally, the reduction of $[CAAC–Au–CAAC]^+$ is discussed, along with the bonding mechanism.

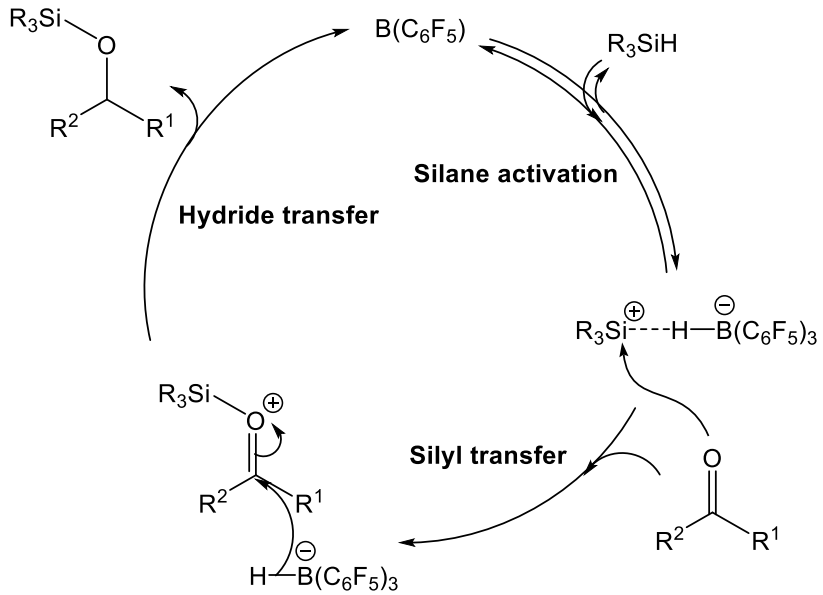
1.1. Frustrated Lewis Pairs

Over the past years the reports of the activation of small molecules via Frustrated Lewis Pairs (FLP) have grown due to the metal-free chemistry. This cleaner method allows for the activation of H_2, CO, CO_2, SO_2 and other small molecules to form relevant reagents in many fields of Chemistry.[1] An FLP consists of a Lewis acid and a Lewis base that cannot combine to form the Lewis adduct due to the steric effects and geometry constraints.[2]

1.1.1. Brief History

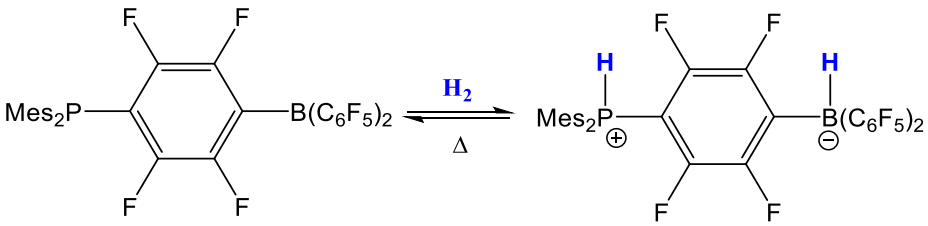
The first report of a ‘frustrated’ dative bond between a Lewis acid and a Lewis base was reported in 1942 by H.C. Brown.[3] He observed that the donor lutidine and the acceptor BMe_3 do not form a classical adduct and he proposed that this anomaly was due to steric congestion. Later, in 1959, Wittig and Benz reported a reaction involving a Lewis base (PPh_3) and a Lewis acid (BPh_3) to give a zwitterionic product $(C_6H_4)(BPh_3)(PPh_3)$.[4] No further reactivity was reported, though this reaction gave a hint for FLP chemistry.

The first recognized FLP reaction, the hydrosilylation of ketones, catalyzed by $B(C_6F_5)_3$, was reported in 1996 by Piers.[5] He showed that $B(C_6F_5)_3$ activated the Si–H bond, followed by a subsequent attack of the ketone to the silane and, finally, a hydride transfer to form the Si–O bond and regenerate the borane (**Scheme 1-1**). The activation of the Si–H bond by a cooperative action of the Lewis base and Lewis acid led to further investigate a combination of Lewis acids and bases that can activate other type of bonds, such as H_2.



Scheme 1-1. Plausible reaction mechanism of the hydrosilylation of ketones catalyzed by $B(C_6F_5)_3$.

The first FLP definition was proposed in 2006. Stefan showed that the activation of H_2 can proceed by the combination of bulky phosphines (e.g. tBu$_3$P, Mes$_3$P) and $B(C_6F_5)_3$.[6] Herein, the steric hindrance prevents to form the dative bond. They also showed that not only the steric hindrance was important to prevent to form the dative bond, but also the geometry constraints in a molecule. The acceptor and donor centers are connected by substituents that do not allow to interact, for example $Mes_2P(C_6F_4)B(C_6F_5)_2$[7] (**Scheme 1-2**) and $Mes_2PCH_2CH_2B(C_6F_5)_2$.[8] The most important remark of these reactions is that $Mes_2P(C_6F_4)B(C_6F_5)_2$[7] reacted reversibly with H_2 under mild conditions. At that time, reversible reactions with H_2 were limited to transition metal complexes (**Scheme 1-2**).



Scheme 1-2. Reaction of $Mes_2P(C_6F_4)B(C_6F_5)_2$ with H_2.

1.1.2. Activation Mechanism

Theoretical calculations have proposed the cooperative action of the Lewis acid and base in activating hydrogen[9,10] or ethylene.[11] Instead the dative bond be 'frustrated' due to steric congestion, computations have revealed the "frustrated complex" is formed via noncovalent interactions.[12] This reactive intermediate is prepared for the incoming H_2 molecule, facilitating the splitting process (**Figure 1-1a**). The frustrated complex was also proposed for FLPs where the link between the donor and acid centers does not allow intramolecular cooperation (**Figure 1-1b**), this is the case for the FLP shown in **Scheme 1-2**. But if the link between centers permits an appropriate arrangement, the FLP may also be able to cleave H_2 in an intramolecular way (**Figure 1-1c**).[9]

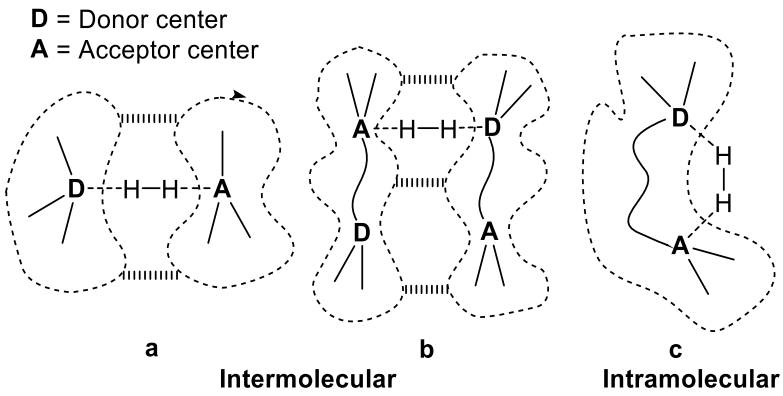


Figure 1-1. Hydrogen splitting by different FLPs: nonlinked pairs (a), linked pairs (b) and with intramolecular preorganization (c). Taken from reference [9].

1.1.3. Role of the basicity and acidity

Pápai and coworkers have studied the thermodynamics of experimentally reported FLP reactions with H_2 using DFT.[13] The calculated reaction free energies were in good agreement with the experimental results, but for a few cases, the theoretical results failed to predict the reversibility of the reaction. To further understand the aspects that take a major role in the FLP chemistry, they proposed to split the calculated reaction free energies into five hypothetical components: the 1) hydrogen cleavage (ΔG_{HH}), 2) preparation (ΔG_{prep}), 3) proton attachment (ΔG_{pa}), 4) hydride attachment (ΔG_{ha}) and 5) stabilization energies (ΔG_{stab}). Its definition is shown in **Figure 1-2b**.

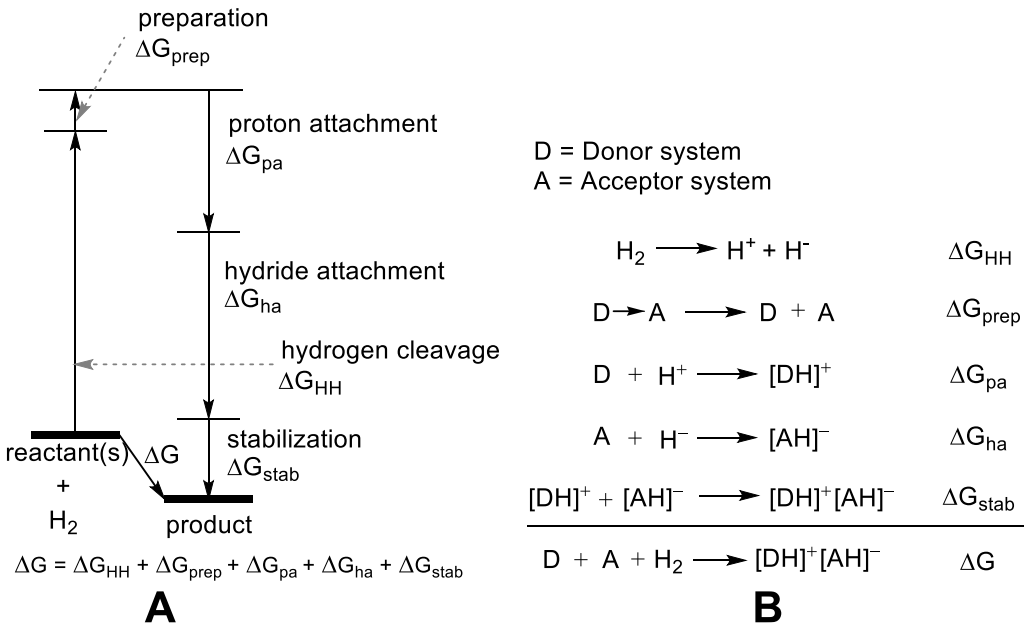


Figure 1-2. Partitioning of the reaction free energy (A) and reaction steps of the partitioning for the Nonlinked FLP (B).

According to the energy decomposition analysis of Pápai and coworkers (**Figure 1-2**), they proposed, as a first step of the thermodynamic cycle, the heterolytic cleavage of dihydrogen into H^+ and H^- ions. The calculated free energy of ΔG_{HH} = +128.8 kcal/mol is highly endergonic which is constant for all FLPs. The second step is the amount of free energy (ΔG_{prep}) needed to break the dative bond between the donor and acceptor centers. But most of the systems do not form a dative bond due to the steric hindrance. In such a case, the ΔG_{prep} becomes cero; for other systems that do form a dative bond, the energy is slightly endergonic. Therefore, it does not contribute in a significant way to the partition scheme. The third and fourth steps are the attachment of a proton (ΔG_{pa}) and a hydride (ΔG_{ha}) and correlate with the basicity and acidity, respectively. These last terms highly contribute to favor the thermodynamics to active H_2. The fifth step, the stabilization energy (ΔG_{stab}), varies in a broader energy interval depending on the FLP. Nonlinked pairs (**Figure 1-1a**) contribute about 10-20 kcal/mol less than linked pairs (**Figure 1-1b**).

From all the partition terms, the attachment of a proton (ΔG_{pa}) and a hydride (ΔG_{ha}) are the most important to favor (or not) the activation of H_2. If the donor contains electron-withdrawing substituents, the ΔG_{pa} increases and does not favor the activation (**Figure 1-3**). For the acceptor centers, highly electron-withdrawing substituents lower the ΔG_{ha} and so the activation is favored (**Figure 1-4**).

From the theoretical calculations of Pápai and coworkers, it is concluded that, in general, strong acceptor centers are needed for activating H_2 when the donor centers are weak. They also pointed out that the use of carbenes in conjunction with a weak acceptor may activate H_2, since the ΔG_{pa} of carbenes are much lower than phosphines (see **carb** in **Figure 1-3**).

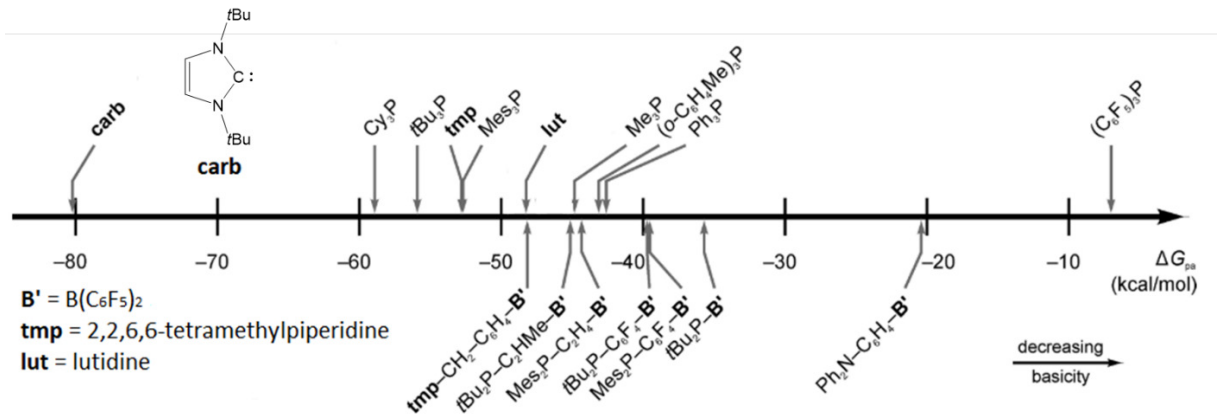


Figure 1-3. Calculated Gibbs free energies of the proton attachment (ΔG_{pa}) to the Lewis donors. Taken from reference [13].

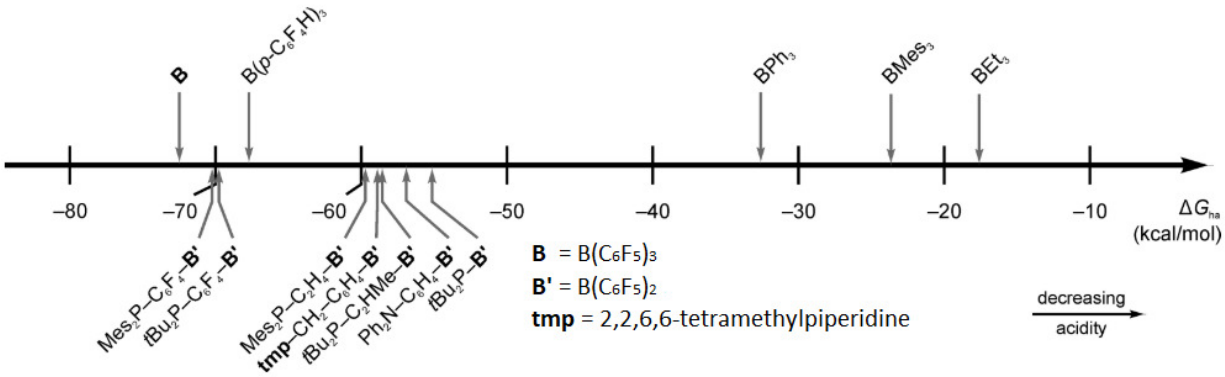
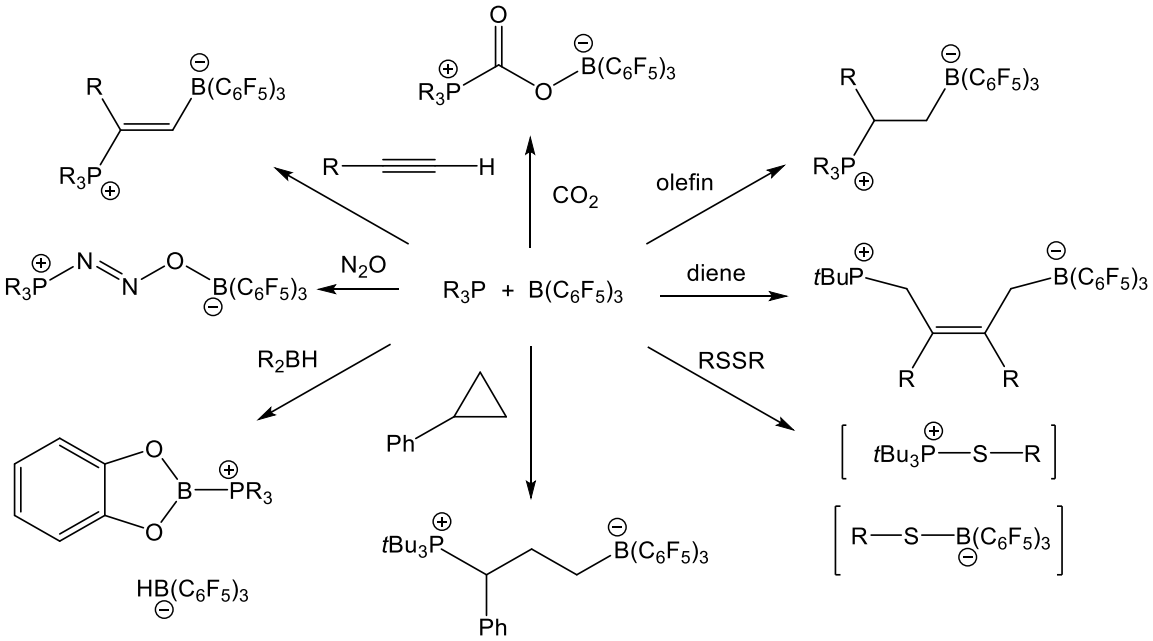


Figure 1-4. Calculated Gibbs free energies of the hydride attachment (ΔG_{ha}) to the Lewis acceptors. Taken from reference [13].

1.1.4. FLP (phosphorus/boron) reactions with small molecules.

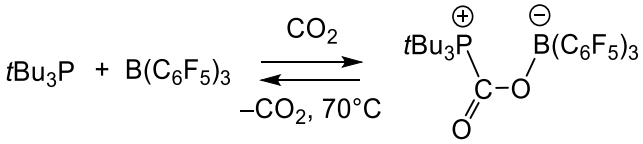
As we have seen, FLPs can activate the strong H–H bond, but the scope of reaction is not limited to activate this bond. In fact, the high reactivity of FLPs can also activate molecules that are of some concern from an environmental standpoint (i.e., CO_2, N_2O, SO_2), giving chemists a great interest in these new reactivity patterns. Some examples of the FLP chemistry with phosphine and borane are given in **Scheme 1-3**.[14]



Scheme 1-3. Examples of FLP chemistry with phoshine/borane combinations.[14]

Reaction with CO_2

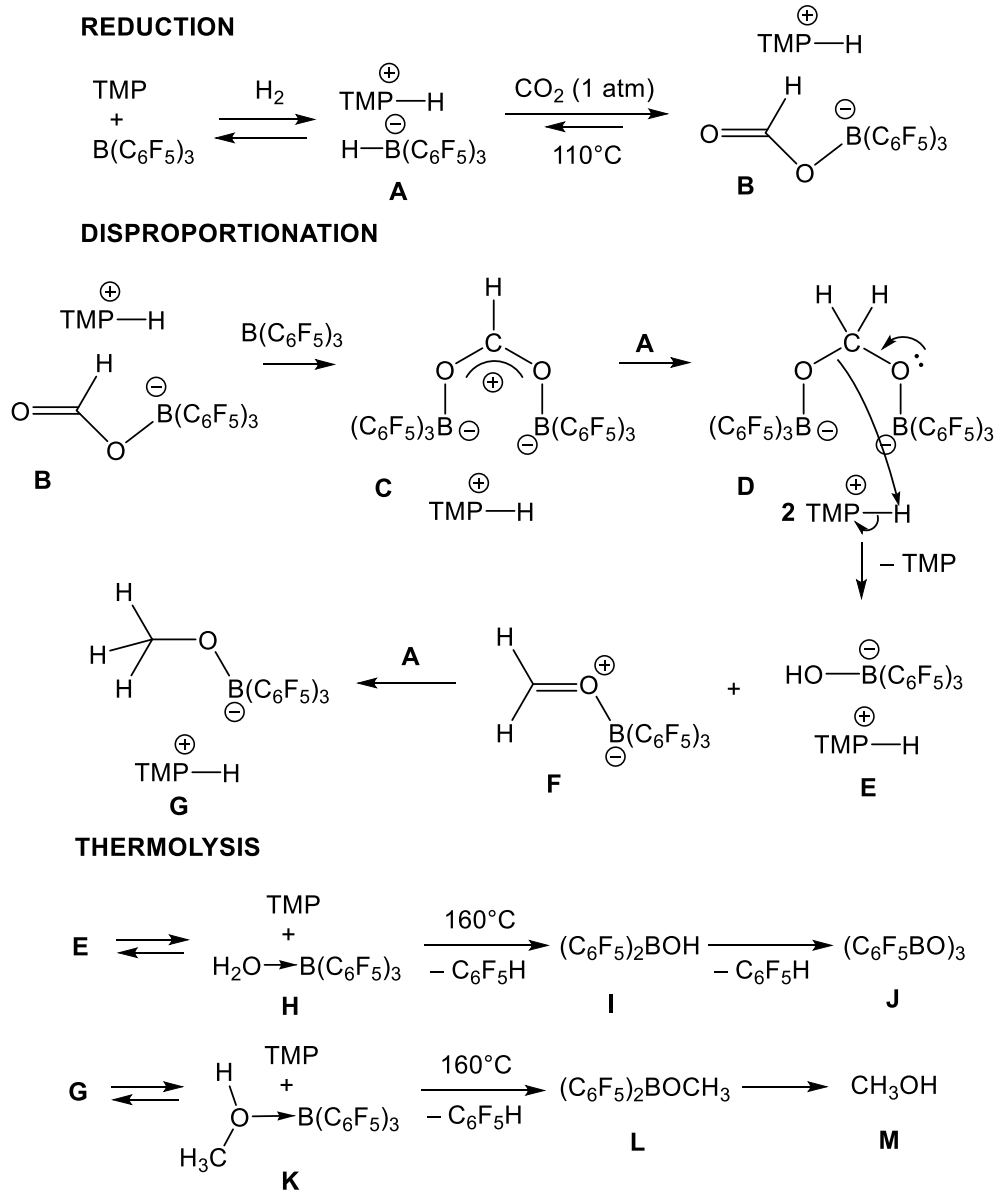
CO_2 is renowned as greenhouse gas so the strategies, to store and confine it, are of growing interest nowadays. Therefore, a big hit came up when it was found that FLP tBu$_3$P/B(C$_6$F$_5$)$_3$ reacted towards CO_2 to give tBu$_3$PCO$_2$B(C$_6$F$_5$)$_3$ (**Scheme 1-4**).[15] This reaction is reversible releasing CO_2 above 70°C.



Scheme 1-4. FLP addition reaction to carbon monoxide.

Another important achievement of the FLP chemistry was the reduction of CO_2 through the use of a FLP, derived from TMP (2,2,6,6-tetramethylpiperidine) and B(C$_6$F$_5$)$_3$, that reacted with CO_2 and H_2.[16] The reaction carries out the conversion of CO_2 to methanol in 24% yield upon heating for 6 days at 160°C. A reaction mechanism was proposed with the experimental data obtained from high-resolution mass spectrometry and NMR spectroscopy (**Scheme 1-5**). First, the TMP and B(C$_6$F$_5$)$_3$ activate H_2 (**A**) followed by the reduction of CO_2 (**B**). All these intermediates are in equilibrium and serve to posterior reactions. Then, the disproportionation of **B** into **G** occurs. Herein, the carbonyl of **B** attacks the B(C$_6$F$_5$)$_3$ Lewis acid (**C**) allowing the carbonyl carbon to increase its acidity. After that, **A** transfer a hydride to give formaldehyde acetal (**D**). This is proposed to be instable in protic media and, therefore, produces **E** and **F**. A

reduction of **F** is achieved via a hydride transfer from **A**. The final step consists of the thermolysis of **E** and **G** at a 160°C producing $(C_6F_5BO)_3$ (**J**) and methanol (**M**).

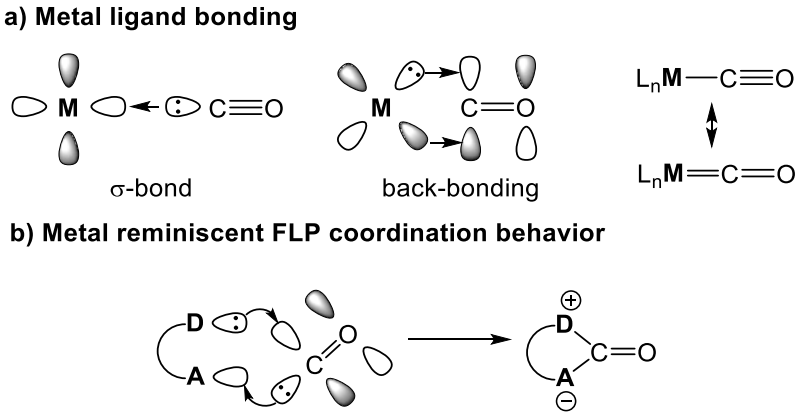


Scheme 1-5. Reaction Mechanism of TMP and $B(C_6F_5)_3$ with H_2 and CO_2.

Reaction with CO

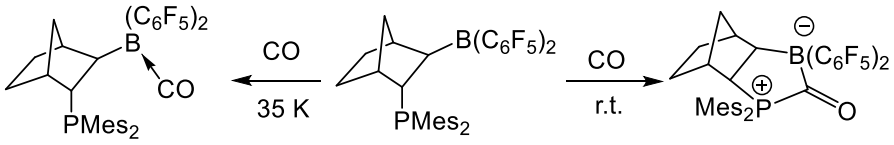
The CO molecule in most of the transition metals serves as a donor and forms a σ-bond with an empty metal-acceptor *d*–orbital and the metal backdonation, in which an occupied metal *d*–orbital interacts with the π* antibonding orbital of CO, strengths the M-C bonding and results in a weakening of the CO bond making it amenable to nucleophilic attacks (**Scheme 1-6a**). In the FLP chemistry, the CO molecule can follow two alternative schemes: addition of CO to the acceptor leads to a simple adduct, or both the acceptor and the donor sites could interact with the CO molecule (**Scheme 1-6b**). This interaction would be reminiscent of a metal-CO bonding, but

instead of the acceptor and donor orbitals located in a single atom, they would be located in different sites.[17]



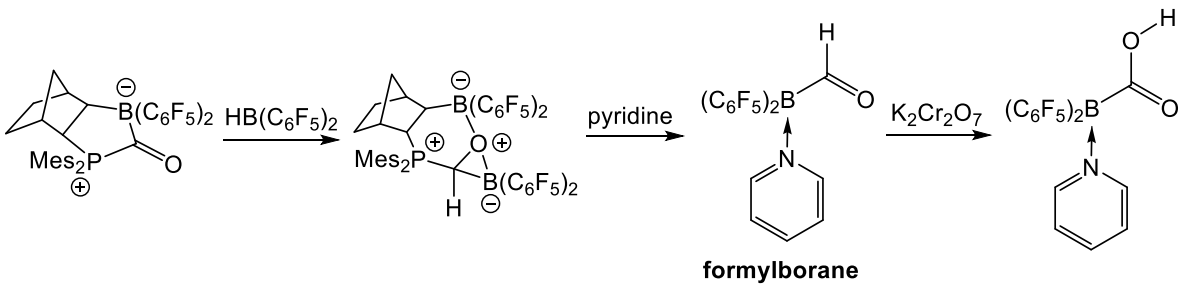
Scheme 1-6. Metal–CO bonding comparison with the FLP bonding scheme.

Reaction of norbornane-based FLP with CO at different temperatures (**Scheme 1-7**) gives an insight of the mechanism: at 35 K or lower, coordination of CO to the acceptor center is only observed and at room temperature the addition product is obtained. Therefore, the reaction occurs stepwise; first, the CO coordinates to the acceptor center followed by the donor attack to the carbon atom.



Scheme 1-7. Norbornane-based FLP addition reaction to carbon monoxide.

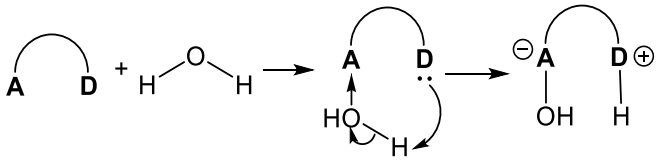
The addition product of the norbornane-based FLP with CO can further react with H–B(C_6F_5)$_2$,[18] but the FLP fragment remains in the molecule (**Scheme 1-8**). One approach to remove the FLP fragment can be achieved with an excess of pyridine liberating formylborane.[18] The stable formylborane is found to be useful in many organic carbonyl reactions[1,19] and can be oxidized to the borane carboxylic acid.[1]



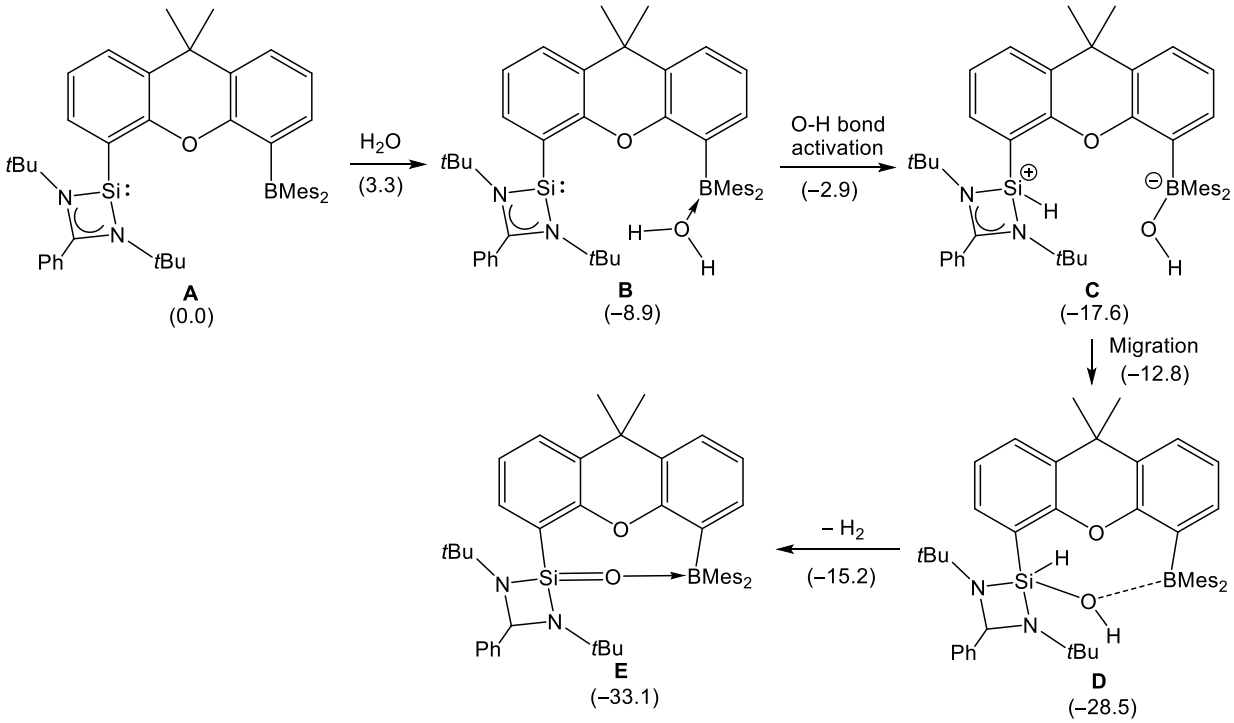
Scheme 1-8. Formation and oxidation reaction of the formylborane.

Reaction with H_2O

The HO–H bond can be easily activated by FLPs. After the coordination of the H_2O into the acceptor center of the FLP, the Lewis base deprotonates the H_2O (**Scheme 1-9**). The reaction generally stops at the HO–H cleavage step, but there is a unique case where a FLP constituted by a silylene and a borane fragment achieves the reduction of water.[20] In **Scheme 1-10** the calculated reaction mechanism is given. As a first step, the water coordinates the borane (**B**), followed by the HO–H activation (**C**). Then, the hydroxyl group of the borane migrates towards the Si center (**D**) and, finally, H_2 is released leaving **E** as a product.



Scheme 1-9. General HO–H bond activation by a FLP.

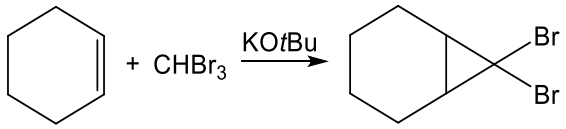


Scheme 1-10. Plausible reaction mechanism of the dihydrogen generation from the reaction of **A** with water. Numbers in parenthesis are relative free energies (in kcal/mol). Numbers below the arrows are the relative free energy of the transition states.

1.2. Carbenes

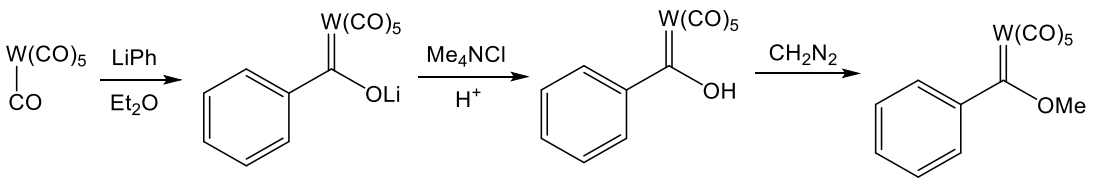
1.2.1. Brief History

In 1855, Geuther and Hermann were studying the alkaline hydrolysis of chloroform.[21] They proposed that this transformation proceeds through a highly reactive intermediate: the dichlorocarbene, a divalent carbon. Nef, in 1897, also proposed the same reaction intermediate for the Reimer-Tiemann reaction and the transformation of pyrrol to α-chloropyridine in chloroform.[22] In both cases, this proposal was not very welcomed by chemists since the divalent carbon was considered as a diradical, and most did not believe in the existence of free radicals at that time as there were no reported examples. It was just through the decades of 1920 and 1930 that the existence of free radicals became established by the community of chemists, and in 1950s there was a resurgent interest in reactions of carbenes. Finally, in 1954, Doering and coworkers proved the existence of a dibromomethylene intermediate in the cyclopropanation reaction where they reacted bromoform and an alkene (**Scheme 1-11**).[23]

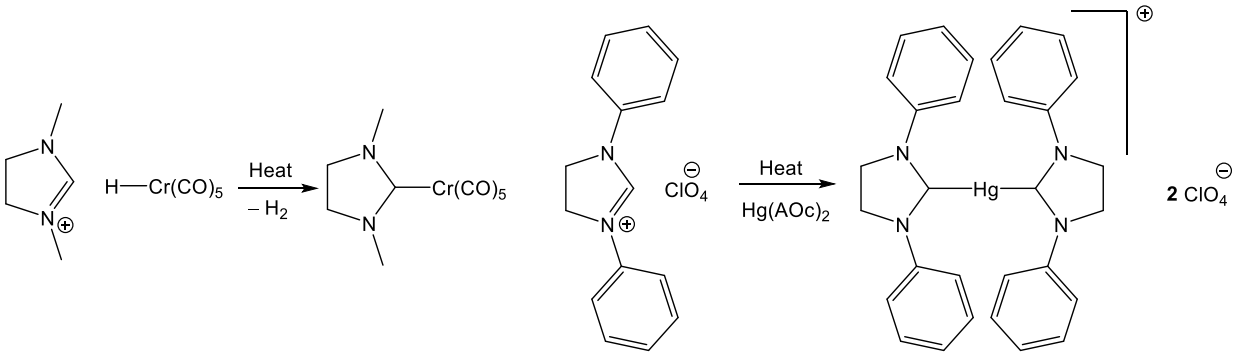


Scheme 1-11. Alkene cyclopropanation via a methylene intermediate.

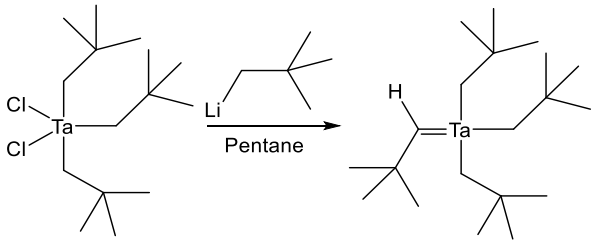
The introduction of the carbenes as ligands in transition metal complexes started in 1964 when Fischer reported and characterized the first metal–carbene complex (**Scheme 1-12**).[24] This chemistry began increasing, and other types of metal–carbenes where synthetized such as the first NHC-metal complex in 1968 by Wanzlick and Ofele (**Scheme 1-13**).[25,26] Schrock then reported the first synthesis of a high oxidation state (d^0) metal-alkylidene complex by and α-abstraction on the tris(2,2-dimethylpropyl)methyl tantalum(V) dichloride precursor (**Scheme 1-14**).[27]



Scheme 1-12. Synthesis of the first recognized metal–carbene complex.



Scheme 1-13. Synthesis of the first NHC-metal complexes.



Scheme 1-14. Synthesis of the first alkylidene-metal (d^0) complex.

1.2.2. Fischer and Schrock-type carbenes

The electronic structure of metal-carbene fragments can be understood by the Dewar-Chatt-Duncanson donor-acceptor model and its representation is shown in **Figure 1-5**.[28] Fischer carbenes have two major orbital interactions between metal and carbene fragment: 1) σ-donation of the carbene ligand to the metal center and 2) π–backdonation from a metal filled *d*-orbital to an empty *p*-orbital of the carbene fragment, and the empty *p*-orbital is further stabilized by the filled *p*-orbital of the adjacent heteroatom (*i.e.* X = O, S, N). Since the carbon of the Fischer carbene holds six valence electrons, the carbon behaves as electrophile. In contrast, Schrock carbenes have a different electronic structure: 1) because no heteroatom stabilizes the *p*-vacant orbital of the carbene, this carbon is defined to be in the triplet state. This allows the carbene to behave as a nucleophile.

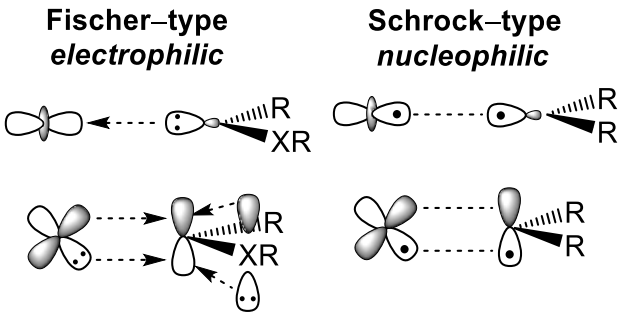


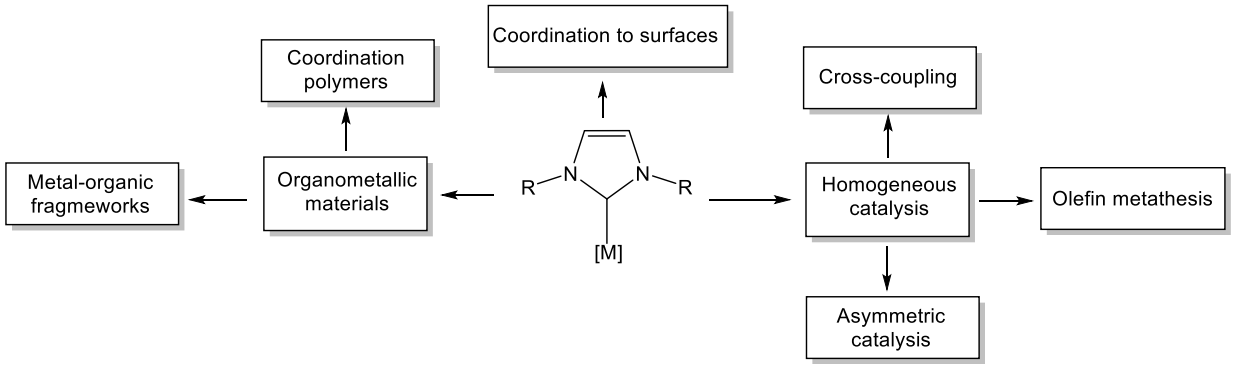
Figure 1-5. Bonding mechanism of Fischer and Schrock-type carbenes.

1.2.3. Heterocyclic carbenes

NHC and CAAC carbenes

In this section, we are interested in studying the N-heterocyclic carbenes (NHCs) and cyclic alkyl(amino) carbenes (CAACs) properties because the results and discussion of this Thesis are related to analogue species of these carbene complexes.

NHCs and CAACs have been employed as strong σ-donating ligands. In general, these carbene ligands have allowed to stabilize low-valent main group elements and transition metals in their low oxidation state.[29,30] Moreover, NHC and CAACs have been shown to function as efficient ligands for transition metals in many fields of chemistry as shown in **Scheme 1-15**.[31]



Scheme 1-15. Applications of NHCs as ligands in metal complexes.

The difference between CAACs and NHCs can be understood by the difference in the σ-donating and π-accepting properties. These are correlated with the energy of the frontier molecular orbitals (FMO):[32] the HOMO and LUMO. Generally, the HOMO corresponds to the carbene lone pair and the LUMO to the antibonding π*($C_{carbene}$–N) orbital. The higher HOMO energy, the stronger σ-donating is the carbene, and the lower LUMO energy the higher π-accepting properties. In CAAC, the HOMO is slightly higher and the LUMO is slightly lower in energy compared with the NHCs (**Figure 1-6**). Therefore, the σ-donation and π-accepting

properties of CAAC are stronger than NHCs.[33] This makes them more suitable for stabilization of chemical species that have not been isolated by employing NHCs as ligands.[34]

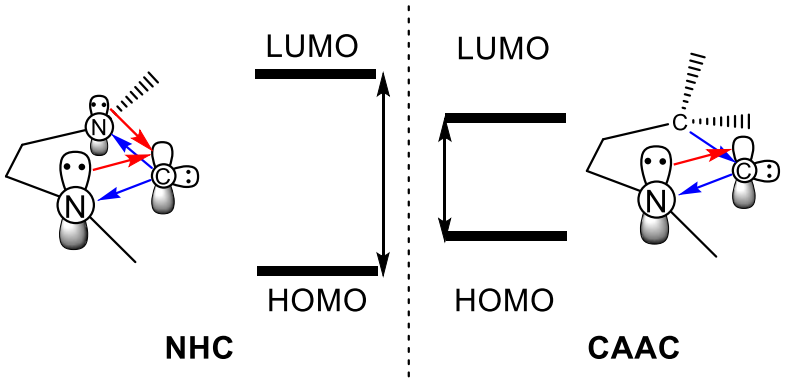


Figure 1-6. Bonding and HOMO-LUMO gap comparison between NHC and CAAC carbenes.

Heterocyclic carbenes containing boron atoms

It has been shown that the π-accepting and σ-donating properties of these carbenes, NHCs and CAACs, are tunable with the introduction of an inorganic backbone.[35] The introduction of a boron atom to the α or β positions can enhance both or one of these properties.[36,37] Theoretical studies were done by Ghambarian and coworkers to understand how these properties change if a boron atom is introduced to a NHC carbene in the α or β positions (**Figure 1-7**).[37] According to their results, the boron-containing NHCs **B** and **C** were calculated more σ-donating and π-accepting than the simple NHC **A**, with **C** being the most σ-donating. The improved σ-donating property of **C** arises from the fact that the boron substituted in the α position is more electropositive than the carbene. This distributes the charge towards the carbon atom making it more σ-donating. The vacant *p*-orbital of the boron atom in the carbenes **B** and **C** allows the lone pair of nitrogen not only to be delocalized in the *p*-orbital of the carbene but also in this new vacant orbital which diminishes the electron population in the *p*-orbital of the carbene and increases the π-accepting properties.

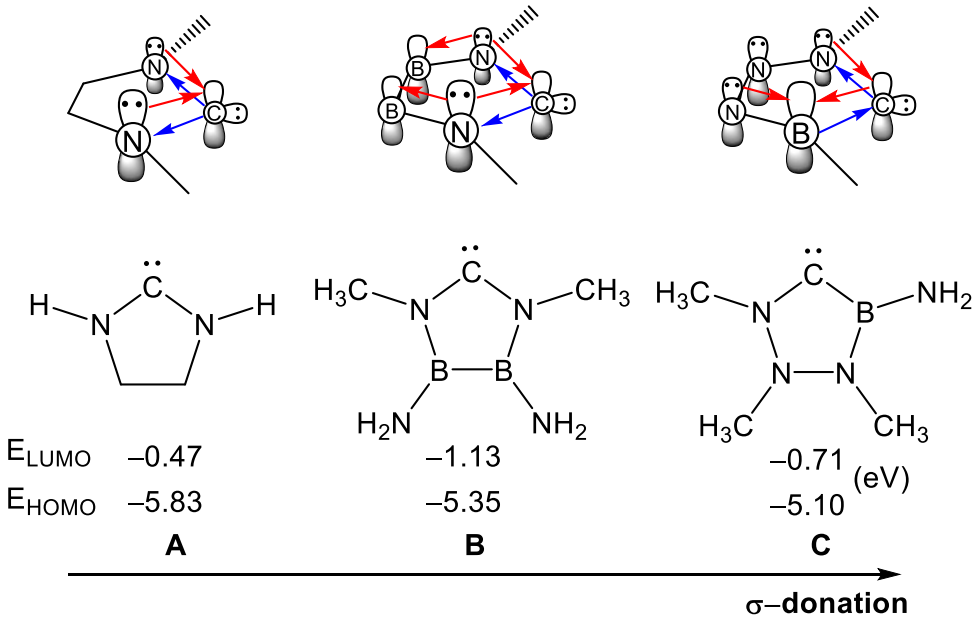


Figure 1-7. Orbital interactions comparison between simple NHC and boron substituted heterocyclic carbenes along with their respective HOMO and LUMO energies (eV).

1.2.4. Gold(I) Carbene Complexes.

Gold(I) carbenes complexes, NHC–Au(I)–L or CAAC–Au(I) –L (L = auxiliary ligand), are one of the main topics of this Thesis. Linear neutral and cationic compounds of this type are widely used in homogeneous catalysis,[43,44] biomedical applications,[45] and as luminescent molecules.[46]

Bonding mechanism of gold carbenes

In 2009, Toste and Goddard proposed a bonding mode of the gold carbene complexes (**Figure 1-1**).[47] They argued that the bonding between the ligand, gold and carbene can be represented as a three-center four-electron σ–hyperbonding; the ligand and the carbene can both donate their lone pair to the vacant 6*s*-orbital of gold (**Figure 1-1**,**A**). The gold center can also backdonate to both ligands from two filled 5*d*-orbitals to the empty acceptor orbitals of the ligand (σ* orbitals for phosphines) and carbene (to its *p*–orbital) (**Figure 1-1**,**B**).

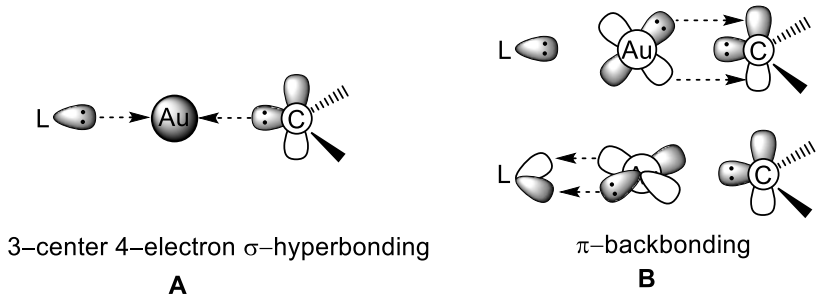
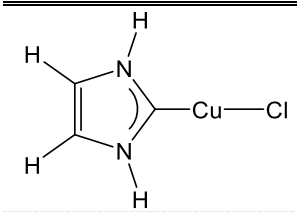
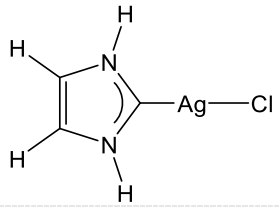
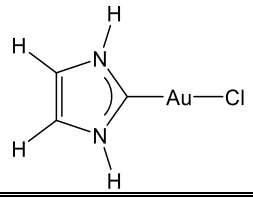


Figure 1-8. Representation of the bonding of gold carbenes complexes.

σ-donating and π-accepting properties

Frenking and coworkers applied the Charge Decomposition Analysis (CDA) approach to NHC copper/silver/gold complexes to measure the σ-donating and π-accepting properties (**Table 1-1**).[48] Their results show that the σ-donating (d) properties is always significantly larger than the π-accepting (b) properties. The ratio d/b of gold (4.35) is the lowest among silver (9.70) and copper (6.64). This can be explained through the strong effect of relativity of gold, which contracts the *s* and *p* orbitals and diffuses the *d* and *f* orbitals.[49]

Table 1-1. CDA results for the NHC-carbene Metal complexes (M = Cu, Ag, Au).

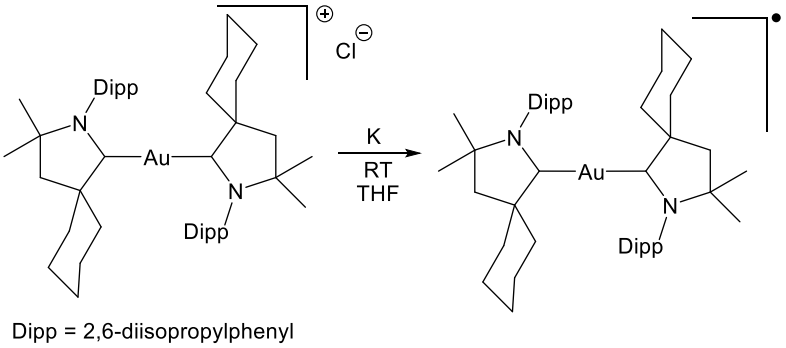
molecule	d[1]	b[2]	d/b[3]
	0.538	0.081	6.64
	0.446	0.046	9.70
	0.396	0.091	4.35

1) Number of electrons donated from carbene to metal, "d", 2) and metal to carbene, "b". 3) d/b represents the ratio.

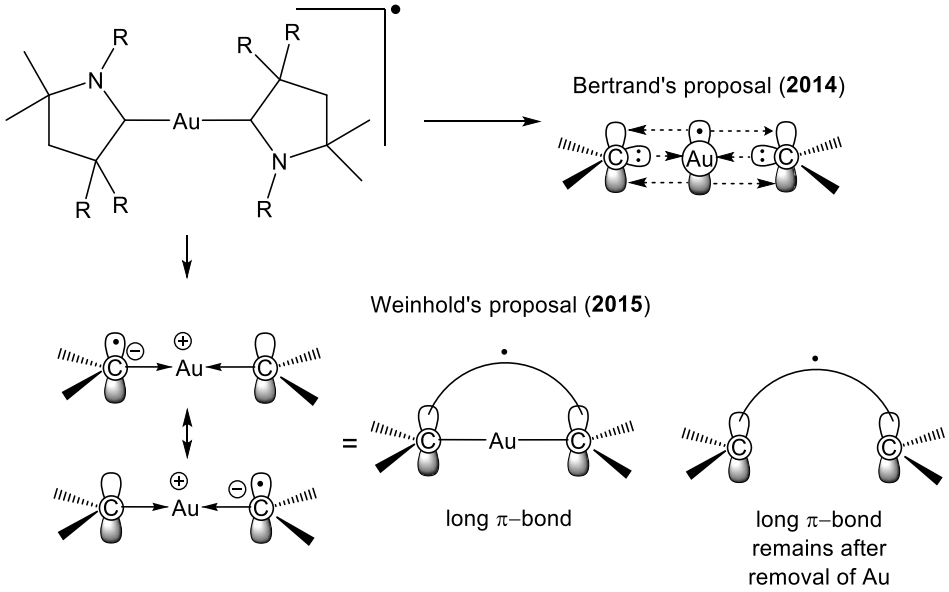
Gold carbene reduction

In 2013, Bertrand reduced the cationic gold complex with two CAAC ligands, $[(CAAC)_2Au]^+$, producing the radical complex, $[(CAAC)_2Au]^{\bullet}$ (**Scheme 1-16**).[50] The uncertainty whether the electron was located in the metal or in the carbene ligand led them, a year later, to carry out a computational study.[51] They suggested that the electron was located in the gold valence 6*p*-orbital giving the electron configuration of gold of $5d^{10}6s^{0}6p^{1}$. With this electron configuration they performed the NOCV calculations, and their results indicated that the unpair electron in the gold atom interacted with the vacant *p*-orbital of carbon carbene; thus, the carbene ligands were more π–acceptor than σ–donor. A year later, in 2015, F. Weinhold corrected the bonding mechanism and stated that previous reported NOCV calculations were wrongly calculated because of their selected reference state.[52] They showed using NBO and a different reference states in NOCV that the reduction fills the vacant *p*-orbital of the carbene with

one electron and this electron can interact with the neighbor vacant *p*-orbital of the other carbon carbene thought a long π–bond. Moreover, they also revealed that the metal can be removed, and the long π-bond remains. Therefore, the inclusion of the *p*-orbital of gold was not necessary for the long π-bonding.



Scheme 1-16. Synthesis of the radical $[(CAAC)_2Au]^{\bullet}$.



Scheme 1-17. Bertrand's and Weinhold's bonding mechanism for the neutral radical $[(CAAC)_2Au]^{\bullet}$.

CHAPTER 2

In this chapter we introduce to the fundaments of quantum mechanics, starting from the Schrödinger equation to the Density Functional Theory. Moreover, Natural Bonding Orbital and Intrinsic Bond Orbitals theories are reviewed.

2.1. Schrödinger Equation

In 1926, Schrödinger postulated the fundamental equation of quantum mechanics. The equation allowed to predict the future behavior of a quantum system. It is a wave equation in terms of a wave function, $\Psi(\vec{\boldsymbol{r}}, t)$, which precisely predicts the probability of events. This wave function contains all the information about this system. Solving the non-relativistic time-dependent Schrödinger equation (Eq. 1) for one particle gives the desired wave function $\Psi(\vec{\boldsymbol{r}}, t)$.[53]

$$i\hbar \frac{\partial}{\partial t}\Psi(\vec{\boldsymbol{r}}, t) = \left[\frac{-\hbar}{2m}\hat{\nabla}^2 + \hat{V}(\vec{\boldsymbol{r}}, t)\right]\Psi(\vec{\boldsymbol{r}}, t) \qquad \text{Eq. 1}$$

The time-independent Schrödinger equation can be derived from the time-dependent Eq. 1.[reference] If the time-dependent wave function $\Psi(\vec{\boldsymbol{r}}, t)$ can be written as a product of a function of time and a function of coordinates, $\Psi(\vec{\boldsymbol{r}}, t)$ becomes

$$\Psi(\vec{\boldsymbol{r}}, t) = f(t)\psi(\vec{\boldsymbol{r}}) \qquad \text{Eq. 2}$$

Thus, the time-independent Schrödinger equation for one particle can be written as

$$\left[\frac{-\hbar^2}{2m}\hat{\nabla}^2 + \hat{V}(\vec{\boldsymbol{r}})\right]\psi(\vec{\boldsymbol{r}}) = E\psi(\vec{\boldsymbol{r}}) \qquad \text{Eq. 3}$$

From Eq. 3 the corresponding Hamiltonian function for a single particle is

$$\hat{H} = \frac{-\hbar^2}{2m}\hat{\nabla}^2 + V(\vec{\boldsymbol{r}}) \qquad \text{Eq. 4}$$

Where the left and right terms are the kinetic, $\hat{T}$, and potential energies, $\hat{V}$

$$\hat{H} = \hat{T} + \hat{V} \qquad \text{Eq. 5}$$

The Hamiltonian above can be derived for N electrons and M nuclei and is written as follows in atomic units

$$\hat{H} = -\sum_{i=1}^{N}\frac{1}{2}\hat{\nabla}_i^2 - \sum_{A=1}^{M}\frac{1}{2M_A}\hat{\nabla}_A^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}} \qquad \text{Eq. 6}$$

Where the first term is the kinetic energy of electrons; the second term is the kinetic energy of the nuclei; the third term represents the Coulomb attraction between electrons and nuclei; the fourth and fifth term are the repulsions between electrons and nuclei.

2.1. Born-Oppenheimer approximation

Since nuclei are heavier than electrons, the electrons can be moving around a fixed nucleus. With this argument we can make a good approximation to Eq. 6, where the second term can be neglected, and the last term can be considered as constant. The remaining terms corresponds to the electronic Hamiltonian describing N electrons in the field of M point charges.

$$\hat{H}_{elec} = -\sum_{i=1}^{N}\frac{1}{2}\hat{\nabla}_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} \qquad \text{Eq. 7}$$

Thus, the Schrödinger equations becomes,

$$\hat{H}_{elec}\psi_{elec} = E_{elec}\psi_{elec} \qquad \text{Eq. 8}$$

The electronic wave function describes the motion of the electrons and depends on the electronic coordinates $\{r_i\}$, but also on the nuclear coordinates $\{R_A\}$, which can select.

$$\psi_{elec} = \psi_{elec}(\{r_i\};\{R_A\}) \qquad \text{Eq. 9}$$

The total energy can be then calculated as,

$$E_{total} = E_{elec} + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}} \qquad \text{Eq. 10}$$

As the electrons move much faster than the nuclei, we can replace the electronic average values, averaged over the electronic wave function,

$$\hat{H}_{nucl} = -\sum_{A=1}^{M}\frac{1}{2M_A}\hat{\nabla}_A^2 + \langle\psi_{elec}|-\sum_{i=1}^{N}\frac{1}{2}\hat{\nabla}_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}} + |\sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}}|\psi_{elec}\rangle = -\sum_{A=1}^{M}\frac{1}{2M_A}\hat{\nabla}_A^2 + E_{total} \qquad \text{Eq. 11}$$

The Schrödinger equation with the nuclear Hamiltonian contains the nuclear wave function which includes the electronic, vibrational, rotational, and translational wave function.

2.2. Hartree-Fock

Approximations to the Schrödinger equations has been a major concern of theoretical chemists. With the Schrödinger equation, only for simple cases, such as H and H_2^+, can be solved exactly.

The main idea of the Hartree-Fock approximation is to use a single Slater determinant, which is antisymmetric with respect to the interchange of the coordinates, to describe the ground state of N electron system,[54,55]

$$|\Psi_o\rangle = |\chi_1\chi_2 \dots \chi_N\rangle \quad \text{Eq. 12}$$

Where $\{\chi_i\}$ are the spin orbitals.

Applying variational principal we get,

$$E_o = \langle\Psi_o|\hat{H}|\Psi_o\rangle \quad \text{Eq. 13}$$

By minimizing E_o with respect the spin orbitals, the Hartree-Fock equation is derived, and has the form of,

$$\hat{f}(i)\chi(x_i) = E_i\chi(x_i) \quad \text{Eq. 14}$$

Where $\hat{f}(i)$ is an effective one-electron operator, known as the Fock operator,

$$\hat{f}(i) = -\frac{1}{2}\hat{\nabla}_i^2 - \sum_{A=1}^{M}\frac{Z_A}{r_{iA}} + v^{HF}(i) \quad \text{Eq. 15}$$

Where $v^{HF}(i)$ is the averaged potential experienced by the ith electron due to the presence of other electrons. Thus, the Hartree-Fock approximation replaces the many-electron problem with a one-electron problem by threating the electron-electron repulsion in an average way.

Further elimination of the spin dependence in Eq. 41 can be done. This lefts only the spatial part, the molecular orbitals $\psi_i(r_1)$.

$$\hat{f}(r_1)\psi_i(r_1) = E_i\psi_i(r_1) \quad \text{Eq. 16}$$

Roothaan showed that the above equation can be solved by introducing a set of spatial basis functions $\{\Phi_i\}$ and expand the unknown molecular orbitals in the linear expansion

$$\psi_i = \sum_{\mu=1}^{K} C_{\mu i}\phi_\mu \quad \text{Eq. 17}$$

Then, the last two equation can derive the integrated Hartree-Fock equation

$$\sum_{v} F_{\mu v}\, C_{vi} = \epsilon_i \sum_{v} S_{\mu v} C_{vi} \qquad \text{Eq. 18}$$

Where $F_{\mu v}$ is an element of the Fock matrix and $S_{\mu v}$ is an element of the overlap matrix.

$$F_{\mu v} = \int dr_1\, \phi_\mu^*(1) \hat{f}(1) \phi_v(1) \qquad \text{Eq. 19}$$

$$S_{\mu v} = \int dr_1 \phi_\mu^*(1) \phi_v(1) \qquad \text{Eq. 20}$$

The above equations can be further analyzed for the closed shell case in which the Fock operator has the form of

$$\hat{f}(1) = \hat{h}(1) + \sum_{a}^{N/2} 2\widehat{J_a}(1) - \widehat{K_a}(1) \qquad \text{Eq. 21}$$

Where $\widehat{J_a}$ and $\widehat{K_a}$ are the closed-shell coulomb and exchange operators.

Combining equations Eq. 21, Eq. 19 and Eq. 17 leads to an expression of the Fock matrix for the closed-shell case

$$F_{\mu v} = \int dr_1\, \phi_\mu^*(1) \hat{h}(1) \phi_v(1) + \sum_{a}^{N/2} \sum_{\lambda\sigma} C_{\lambda a} C_{\sigma a}^* [2(\mu v|\sigma\lambda) - (\mu\lambda|\sigma\lambda)] \qquad \text{Eq. 22}$$

The first term can be defined as the core-Hamiltonian matrix

$$H_{\mu v}^{core} = \int dr_1\, \phi_\mu^*(1) \hat{h}(1) \phi_v(1) \qquad \text{Eq. 23}$$

And in the second term, the density matrix can be introduced

$$P_{\mu v} = 2 \sum_{a}^{N/2} C_{\mu a} C_{va}^* \qquad \text{Eq. 24}$$

Therefore, Eq. 23 and Eq. 24 can be introduced into the Fock matrix Eq. 22

$$F_{\mu v} = H_{\mu v}^{core} + \sum_{\lambda\sigma} P_{\mu v} [(\mu v|\sigma\lambda) - \frac{1}{2}(\mu\lambda|\sigma\lambda)] \qquad \text{Eq. 25}$$

$$G_{\mu v} = \sum_{\lambda\sigma} P_{\mu v} [(\mu v|\sigma\lambda) - \frac{1}{2}(\mu\lambda|\sigma\lambda)] \qquad \text{Eq. 26}$$

$$F_{\mu v} = H_{\mu v}^{core} + G_{\mu v} \qquad \text{Eq. 27}$$

Where $G_{\mu v}$ is the two-electron part of the Fock matrix.

Because the Fock matrix depends on the density matrix or in the expansion coefficients, the Roothaan equations are nonlinear. Thus, they must be solved iterative way, known as the self-consistent field method (SCF).

2.3.Self-Consistent Field

With the previous derived equations in the Hartree-Fock section it is possible to obtain a restricted closed-shell Hartree-Fock wave functions. As the equations are non-linear, they are solved using the self-consistent field procedure (SCF), which can be applied as follows:[54]

1. Define the nuclear coordinates $\{R_A\}$, atomic numbers $\{Z_A\}$, number of electrons (N) and the basis set $\{\Phi_i\}$.
2. Calculate the integrals of the elements of the overlap matrix (Eq. 20), $S_{\mu\nu}$, core-Hamiltonian matrix (Eq. 23), $H_{\mu\nu}^{core}$, and the two-electron integrals, $(\mu\nu|\sigma\lambda)$.
3. Diagonalize the overlap matrix, **S**, and transform to a **X** matrix either using a symmetric (Eq. 28) or canonical orthogonalization (Eq. 29).

$$\boldsymbol{X = Us^{-1/2}U^{\dagger}} \qquad \text{Eq. 28}$$

$$\boldsymbol{X = Us^{-1/2}} \qquad \text{Eq. 29}$$

4. Obtain a guess at the density matrix **P** (Eq. 24**)**.
5. Calculate the two-electron matrix **G** (Eq. 26) from the formed density matrix **P**.
6. Calculate the Fock matrix with the **G** and $H_{\mu\nu}^{core}$ matrices (Eq. 27).
7. Determine the transformed Fock matrix $\boldsymbol{F' = X^{\dagger}FX}$**.**
8. Diagonalize **F'** to obtain **C'** and ϵ.
9. Evaluate $\boldsymbol{C = XC'}$.
10. Form a new **P** density matrix from the obtained **C** (Eq. 24).
11. Determine if the procedure has converged, if not return to step 5.

2.4. Density Functional Theory

Density Functional Theory (DFT) is a reformulation of the Schrödinger equation done by Hohenberg and Kohn in 1964.[56] Their first theorem established that, for molecules with no degenerate ground states, the energy of the ground state, the wave function and other electronic properties can be determined by the electron density in that state. Thus, the energy of the ground state, E_o, is the functional of the electron density.[56]

$$E_o = E_o[\rho_o] \qquad \text{Eq. 30}$$

The electron density is defined as:

$$\rho(\vec{\boldsymbol{r}}) = N \sum_{ms_1} \dots \sum_{ms_N} \int \dots \int |\psi(\vec{\boldsymbol{r}}, ms_1, \dots, \overrightarrow{\boldsymbol{r_N}}, ms_N|^2 d\boldsymbol{r_2} \dots d\boldsymbol{r_N} \qquad \text{Eq. 31}$$

The electron density is the probability of finding an electron in **r** with any spin. Because of the complexity for solving the exact DFT equation, Hohenberg and Kohn divided the electron density into one part of non-interacting particles and the other treated like corrections to the free electron-gas energy.[56] It can be written as:

$$E[\rho(\vec{\boldsymbol{r}})] = T[\rho(\vec{\boldsymbol{r}})] + J[\rho(\vec{\boldsymbol{r}})] + E_{xc}[\rho(\vec{\boldsymbol{r}})] + v[\rho(\vec{\boldsymbol{r}})] \qquad \text{Eq. 32}$$

Where $T[\rho(\vec{\boldsymbol{r}})]$ is the kinetic energy functional, $J[\rho(\vec{\boldsymbol{r}})]$ the Coulomb functional, $E_{xc}[\rho(\vec{\boldsymbol{r}})]$ the exchange-correlation functional and $v[\rho(\vec{\boldsymbol{r}})]$ the effective potential energy functional. The first, second and fourth terms can be calculated accurately as follows:

$$T[\rho(\vec{\boldsymbol{r}})] = -\frac{1}{2}\int \sum_{i=1}^{N} |\nabla \varphi_i(\vec{\boldsymbol{r}})|^2 \, d\vec{\boldsymbol{r}} \qquad \text{Eq. 33}$$

$$v[\rho(\vec{\boldsymbol{r}})] = \int v^{ext}(\vec{\boldsymbol{r}})\rho(\vec{\boldsymbol{r}}) d\vec{\boldsymbol{r}} \qquad \text{Eq. 34}$$

$$J[\rho(\vec{\boldsymbol{r}})] = \int\int \frac{\rho(\vec{\boldsymbol{r}})\rho(\vec{\boldsymbol{r}}')}{|\vec{\boldsymbol{r}} - \vec{\boldsymbol{r}}'|} d\vec{\boldsymbol{r}} d\vec{\boldsymbol{r}}' \qquad \text{Eq. 35}$$

For the exchange-correlation functional, no equation was written, because it does not have an exact form. To find this functional, an approximation must be done. Each density functional approximates the exchange-correlation functional in different ways which defines the degree of precision.

To solve the many-electron problem in DFT, molecular orbitals were introduced again in the free-electron gas model, where the electron density is defined as:

$$\rho(\vec{\boldsymbol{r}}) = \sum_{i=1}^{N} |\psi_i(\vec{\boldsymbol{r}})|^2 \qquad \text{Eq. 36}$$

After applying the variational method to the energy functional (Eq. 32), the Kohn-Sham equations are obtained.

$$\begin{gathered}
\left[-\frac{\nabla^2}{2} + v^{ext}(\vec{\boldsymbol{r}}) + J + V_{xc}\right]\psi_1(\vec{\boldsymbol{r}}) = E_1\psi_1(\vec{\boldsymbol{r}}) \\
\left[-\frac{\nabla^2}{2} + v^{ext}(\vec{\boldsymbol{r}}) + J + V_{xc}\right]\psi_2(\vec{\boldsymbol{r}}) = E_2\psi_2(\vec{\boldsymbol{r}}) \\
\vdots \\
\left[-\frac{\nabla^2}{2} + v^{ext}(\vec{\boldsymbol{r}}) + J + V_{xc}\right]\psi_N(\vec{\boldsymbol{r}}) = E_N\psi_N(\vec{\boldsymbol{r}})
\end{gathered} \qquad \text{Eq. 37}$$

2.5. Transition State Theory

In 1935 Eyring and Polanyi develop a theory to estimate reaction rates of elementary chemical reactions. The famous Eyring's equation (Eq. 38) has been applied succesfully to a variety of rate processes.[57]

$$k = \frac{k_B T}{h} \frac{Q^{\ddagger}}{Q_A Q_B} e^{\frac{-E_o}{RT}} \qquad \text{Eq. 38}$$

Where k is the reaction rate constant, T the temperature, E_o free energy of activation, R gas constant, k_B Boltzmann constant, h Planck's constant and $Q^{\ddagger}$, Q_A, Q_B are the partition functions of the transition state and the reactants, respectively.

The most important features of this theory are:[58]

1. The reaction rates can be calculated by only knowing the activated complexes, which lie at the saddle point of the potential energy surface (PES). The details before the activated complexes are achieved are not necessary for obtaining the overall rate.
2. The activated complex is in a state of "quasi-equilibrium" with the reactants.
3. The motion of the system at the saddle point, along a reaction coordinate, can be treated as free translational motion.

2.6. Natural Bond Orbitals

The NBO theory transforms the many-electron molecular wavefunction to a Lewis structure picture that best describes the molecule in terms of localized one-center (lone pair) and two-center (bond) elements, making NBO chemically intuitive.[59] The delocalization effects appear as a deviations of this Lewis structure (non-Lewis), allowing to calculate the interaction energies between a occupied and a vacant orbital.[59]

The NBO method makes use of only the first-order reduced density matrix of the wavefunction, $\Gamma^{(1)}$, and so it can be applied to wavefunctions of general mathematical form. [59] The importance of NBO using this matrix comes from the fact that the first- and second-order density matrices $\Gamma^{(1)}$, $\Gamma^{(2)}$ are needed to measure any property of a pure-state molecular species. But from these two matrices, only $\Gamma^{(1)}$ would be necessary if the correlations effects were completely negligible. Thus, the $\Gamma^{(1)}$ is more important than $\Gamma^{(2)}$.[59]

Because $\Gamma^{(1)}$ is a one-electron operator, it is deeply connected to orbital-level description of the N-electron system as described in the following equation:

$$\Gamma^{(1)}\theta_i = n_i\theta_i, \quad i = 1,2,\dots,N \qquad \text{Eq. 39}$$

Where θ_i is the natural orbital (NO) and n_i its occupancy. Thus, the natural orbitals (NOs) are eigenvectors of $\Gamma^{(1)}$. [60]

The set of natural orbitals $\{\theta_i\}$ provides the most compact and rapidly convergent description of all one-electron properties of the wavefunction Ψ. One can define the NOs as the

"orbitals selected by the wavefunction itself (through its reduced $\Gamma^{(1)}$) as optimal for its own description". [59]

The occupation of NOs is not restricted to integer values, as for the Molecular Orbitals (MOs), but can vary in range from 0 to 2 in the case of closed-sell spatial orbitals. However, the NOs are chosen to have the greatest condensation of electron density into the fewest orbitals so the eigenvalue Eq. 39 can be satisfied. Because of this maximum-occupancy property, one can search for localized (i.e. 1- or 2-center) regions that contain high-occupancy "local NOs", expecting that such regions are associated with electron pairs in the Lewis dot diagram.

F. Weinhold and J. P. Foster demonstrated that the density matrix and the natural orbitals can be generalized to identify optimal local bonding patterns related to a Lewis structure picture, leading to the known "natural bond orbitals" that correspond to a localized description of the electron density.[61] The NBOs have almost near double-occupancy, with slight deviations that reflect the slight resonance effects of the molecule, giving a chemical intuitive description of the bonding pattern.[59]

2.6.1. E(2) Second Order Perturbation Theory

The E(2)s are the energies related to the interaction between a donor and acceptor NBO orbitals. Even though these values are unmeasurable and have no direct physical significance, they correlate with a variety of trends in chemical bonding and reactivity, and therefore can help in understanding experimental or computational data.[59]

To know how these energies are obtained, consider that the total wavefunction Ψ can be composed of a Lewis-type $\Psi^{(L)}$ and a non-Lewis contribution $\Psi^{(NL)}$,[59]

$$\Psi = \Psi^{(L)} + \Psi^{(NL)} \qquad \text{Eq. 40}$$

Where $\Psi^{(L)}$ is known and is related to an idealized Lewis structure in which each NBO has exact double occupancy because it has no delocalization effects, and $\Psi^{(NL)}$ is unknown and is related to departures of the idealized Lewis structure. [59]

Now assume a corresponding Hamiltonian $\hat{H}$ that can be compose of the Lewis $\hat{H}^{(L)}$ and non-Lewis Hamiltonian $\hat{H}^{(NL)}$,[59]

$$\hat{H} = \hat{H}^{(L)} + \hat{H}^{(NL)} \qquad \text{Eq. 41}$$

Given these two last equations (Eq. 40 and Eq. 41) and the form of the Schrödinger equations(Eq. 8), $\hat{H}\Psi = E\Psi$, there must exists an energy of the system, E, such that

$$E = E^{(L)} + E^{(NL)} \qquad \text{Eq. 42}$$

As the Lewis-type Hamiltonian operator $\hat{H}^{(L)}$ has a known eigenvector $\Psi^{(L)}$ and eigenvalue $E^{(L)}$ a "systematic perturbation theory" analysis can be started from the last three

equations. Thus, adding the perturbation, the non-Lewis Hamiltonian, $\widehat{H}^{(NL)}$ to the unperturbed Lewis Hamiltonian $\widehat{H}^{(L)}$ leading to a total Hamiltonian $\widehat{H}$ that accounts for the delocalization effects of the idealized Lewis structure (Eq. 41). This perturbation is constrained to second-order because of the high accuracy description of the Lewis-wavefunction $\Psi^{(L)}$ (almost 99% of the description of the electron density ρ_L).[59]

Moreover, in the resonance-free Lewis structures, the donor $\{\Omega_i^{(L)}\}$ and acceptor NBOs $\{\Omega_i^{(NL)}\}$ have no interaction due to their mutual orthogonality (Eq. 43),

$$\int \Omega_i^{(L)*} h^{(0)} \Omega_j^{(NL)} d\tau = 0 \qquad \text{Eq. 43}$$

However the effective 1e-Hamiltonian operator F (Fock, Kohn-Sham or related) has non-vanishing donor-acceptor interactions (Eq. 44),

$$F_{ij} = \int \Omega_i^{(L)*} F \Omega_j^{(NL)} d\tau \neq 0 \qquad \text{Eq. 44}$$

This last term appears in the energy results, $\Delta E_{ij}^{(2)}$ (also known as E(2)), obtained by the perturbation method constrained to second-order (Eq. 45),

$$\Delta E_{ij}^{(2)} = \frac{-q_i \left|F_{ij}\right|^2}{\left(\epsilon_j^{(NL)} - \epsilon_i^{(L)}\right)} \qquad \text{Eq. 45}$$

Where q_i is the occupancy of the donor orbital, and $\epsilon_i^{(L)}$, $\epsilon_j^{(NL)}$ are the donor and acceptor orbital energies respectively.

In general, the mixing of donor and acceptor orbitals lead to an overall energy lowering, $\Delta E_{ij}^{(2)}$ or E(2), ("stabilization") of the new mixed orbital (**Figure 2-1**).

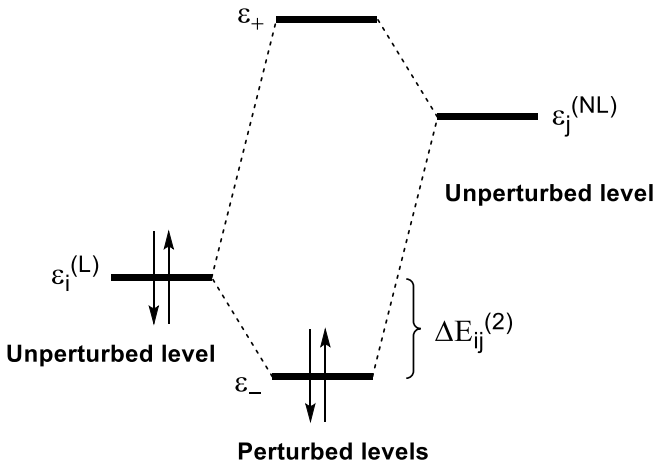


Figure 2-1. Stabilizing interaction between a filled donor NBO orbital and a vacant acceptor orbital.

2.7. Intrinsic Bond Orbitals

Intrinsic Bond Orbitals (IBO) method is commonly used to understand chemical bonds or the electron-flow through an intrinsic reaction coordinate (IRC).[62] This method connects the quantitative self-consistent field (SCF) wavefunctions to a qualitative chemical picture, achieved without empirical input, that is described through the bonds named IBOs. The best of this method is that the known Lewis structure of molecules emerge from the IBOs.[62]

Commonly, the basis functions used to calculate Molecular Orbitals (MOs) are more complex than the minimal basis sets given for an atom, for example a minimal basis for carbon would only contain atomic orbitals (AOs) 1s, 2s, $2p_x$-$2p_z$. The calculated MOs derived from an accurately calculated wavefunction are complicated to understand because they cannot be clearly associated with any atom. On the other hand, the MOs could be calculated from a minimal basis of free-atom AOs and would be easy to comprehend, but the calculated wavefunction would be inaccurate because the AOs contain no polarization due to the molecular environment. An approach to overcome this consist in determining a set of polarized AOs, termed intrinsic atomic orbitals (IAOs), which can exactly describe the MOs.[63]

The IAOs are obtained by projection of the occupied Molecular Orbitals, obtained from an accurate calculated wavefunction, onto pre-computed AOs from Hartree-Fock calculations on the isolated atoms with the proper basis sets (i.e. def2-SVP).[63]

To further explain this, let

$$P_{12} = \sum_{\mu\nu \,\epsilon\, B_1} |\mu\rangle S^{\mu\nu} \langle\nu| \quad P_{21} = \sum_{\rho\sigma \,\epsilon\, B_2} |\rho\rangle S^{\rho\sigma} \langle\sigma| \qquad \text{Eq. 46}$$

Denote the projectors onto the bases B_1 and B_2 that correspond to a large basis set and a minimal basis set of a free atom respectively, where $S^{\mu\nu}/S^{\rho\sigma}$ are inverse overlap matrices in B_1/B_2. [63] Then the depolarized MOs $\{|i\tilde{}\rangle\}$

$$\{|i\tilde{}\rangle\} = orth\{P_{12}P_{21}|i\rangle\} \qquad \text{Eq. 47}$$

are obtained by projecting the accurate MOs $|i\rangle$ from the main basis B_1 into the minimal basis B_2 (which does not express polatization) and back. The depolarized molecular lies completely within the space spanned by free-atom AOs $|\rho\tilde{}\rangle$ $\{P_{12}|\rho\tilde{}\rangle, |\rho\tilde{}\rangle \,\epsilon\, B_2\}$, and thus, they can be divided into a set of occupied and virtual valence orbitals. Finally, the polarized AOs $|\rho\rangle$ or IBOs can be generated from the free-atom AOs $|\rho\tilde{}\rangle$ by simply projecting their contributions in the depolarized occupied space $O\tilde{} = \sum_{i\tilde{}} |i\tilde{}\rangle\langle i\tilde{}|$ and its complement $1 - O\tilde{}$ into their polarized counter parts $O = \sum_i |i\rangle\langle i|$: [63]

$$|\rho\rangle = \left(OO\tilde{} + (1-O)(1-O\tilde{})\right)P_{12}|\rho\tilde{}\rangle \qquad \text{Eq. 48}$$

2.8. Computational methodology

All the electronic structure calculations were performed using Gaussian09 rev. C.01 package.[64] Geometry optimizations were carried out with the long-range hybrid functional ωB97XB–D[65] in conjunction with the Pople's 6-311G(d) triple-ζ quality basis set with one polarization function. Subsequent harmonic frequency calculations were computed to corroborate the character of each optimized species. Depending on the number of negative eigenvalues of the hessian matrix, it is possible to classify each optimized structure as minimum (zero) or transition state (only one). Thermal and entropy corrections to the total energy were taken from the thermochemistry analyses in the output file at 298K and 1 atm unless otherwise specified.

The solvation effects added to the electronic Hamiltonian were taken into consideration by performing single-point calculations over the optimized geometries at the ωB97XB–D/6-311g(d) level of theory using the PCM[66] model using the SMD[67] parameters according to the Truhlar's model with benzene as solvent (ε = 2.2706). These energies were added to the gas-phase calculations and are reported as the final energy values. Therefore, the final reported energy values are in solvent-phase calculated at the SMD(benzene): ωB97XB–D/6-311G(d).

Moreover, the NBO7.0.6 program[68] was used to analyze the bonding mechanism of the chemical structures obtained, and the IBO program (v20211019-RevA) [63] for plotting the intrinsic bond orbitals. All NBO and IBO calculations were performed as single points over the optimized structures. IBO calculations were computed at a different level of theory: PBE/def2-SV(P). This is because all the calculations could only be performed in a normal computer, not in a supercomputer. A higher level of theory required larger amounts of RAM memory, which the computer did not have.

AICD software version 3.0.4[69,70] was employed to compute the "Anisotropy of the Induced Current Density (AICD)" to determine if the system is non-aromatic, aromatic and anti-aromatic. Nucleus-Independent Chemical Shifts (NICS) profiles were also performed for the same purpose.[71] All these calculations used the level of theory: SMD(benzene): ωB97XB–D/6-311G(d).

Hypothesis of this Work

- A second borane in a Frustrated Lewis Pair (FLP), formed by a borane and a phosphine, confers a different reactivity with CO, H_2O and other small molecules than with FLP without this second borane.

- The π–accepting σ–donating properties of the new BNC carbene gold(I) complexes produced by the reaction of an azadiboriridine and isocyanide are better compared with CAAC and NHC gold(I) complexes.

General Objective

Two new boron ligands are studied in this thesis. The first ligand is related to the FLP chemistry: the bisborane-phosphine. The objective here is to understand the reactivity, via density functional theory, of this new FLP with small molecules (H_2O, H_2, CO, R-OH). The bisborane-phosphine contains two boranes instead of one, which enhances the reactivity compared with normal borane-phosphine FLPs. The second ligand is related to the boron-containing heterocyclic carbenes (BCN). The objective is to study the electronic structure and compare it with conventional heterocyclic carbenes (such as: CAAC, NHC) predicting its σ–donating and π–accepting properties. Finally, all of this results are supported by experimental data given from the Dr. Rong Shang research group.

Specific Goals

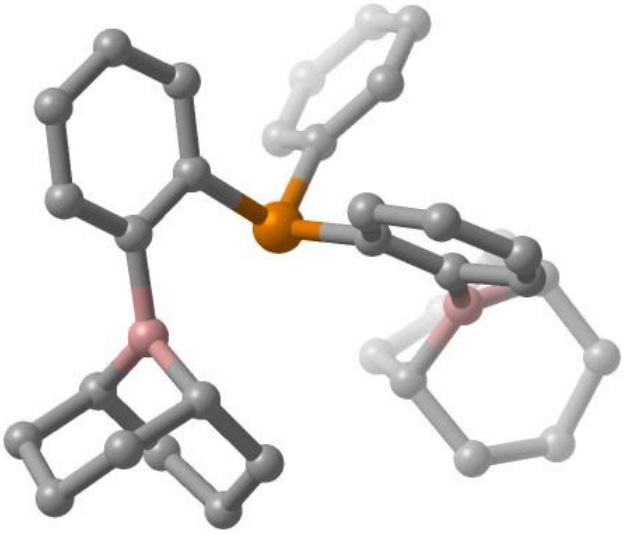
1. To propose and calculate intermediates of each plausible reaction mechanism.
2. To find transition states that connects the proposed intermediates.
3. To analyze if the reaction mechanism is plausible according to the calculated energetic profile.
4. To analyze the electronic structure of chemical structures that the bonding pattern is unclear by using quantum-mechanical softwares.
5. To compare the theoretical results with the experimental ones provided by the Dr. Rong Shang research group from the University of Hiroshima.

Justification

The chemistry of FLP has been increasing over the last year because it can do reactions that only the transition metals did; activating H_2, CO_2, and other small molecules. However, there is lack of information to FLPs with one phosphine and two boranes. This second borane gives other features to FLP, further developing the FLP chemistry.

Boron containing carbenes have been recently studied and have shown to have better π–accepting and σ–donating properties than the CAAC and NHC carbenes. However, some of this carbenes are proposed theoretically. Herein, the reaction mechanism and the electronic structure of a synthetized Boron containing carbene bonded to a gold(I) metal is studied. This leads to further develop new boron carbene complexes.

CHAPTER 3



This chapter focus on the study of reactivity of the bisborane-phosphine Frustrated Lewis Pair (FLP) with small molecules such as H_2, H_2O, CO. This new FLP contains two acid legs, boranes, and one base center, a phosphine (**Figure 3-1**) which gives it a new reactivity compared with the simple borane-phosphine FLP. For simplicity, this FLP is referred as BPB compound. Most of these calculations are compared with the experimental data provided by Dr. Rong Shang's students, Takumi Oishi and Yichuan Jing from the University of Hiroshima. In the first section, the reaction of the first isolated bisborane-phosphine FLP by Dr. Rong Shang research group with the proposed small molecules is studied. This FLP contains the boryls: 9-Borabicyclo[3.3.1]nonan-9-yls. As it will be shown, its reactivity with H_2O and CO is quite different than for conventional FLPs; it can reduce H_2O to H_2. In the second section, another bisborane-phosphine FLP derivate is studied but now the borane contains cyclohexyl (Cy) substituents. These substituents confer a different reactivity towards the small molecules H_2O and CO because other products are observed. The reaction mechanism is not yet completed and therefore, we used as model the reaction mechanism of the first FLP to calculate for the other FLP derivative.

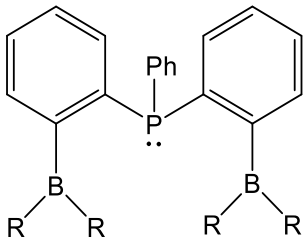


Figure 3-1. bisborane-phosphine Frustrated Lewis Pair.

3.1. bisborane-Phosphine BPB 3-BBN

We first present the study of the bisborane-phosphine FLP substituted with 9-borabicyclo[3.3.1]nonan-9-yls(**Figure 3-2**). This borane ligand is bulky enough to prevent the formation of the P–B bond and because of the double FLP, the reaction with small molecules is often different than other FLPs containing phosphine and borane (FLP (P/B)).

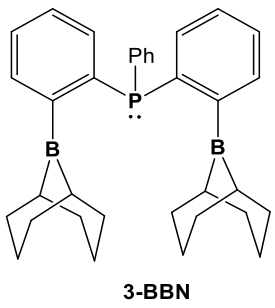


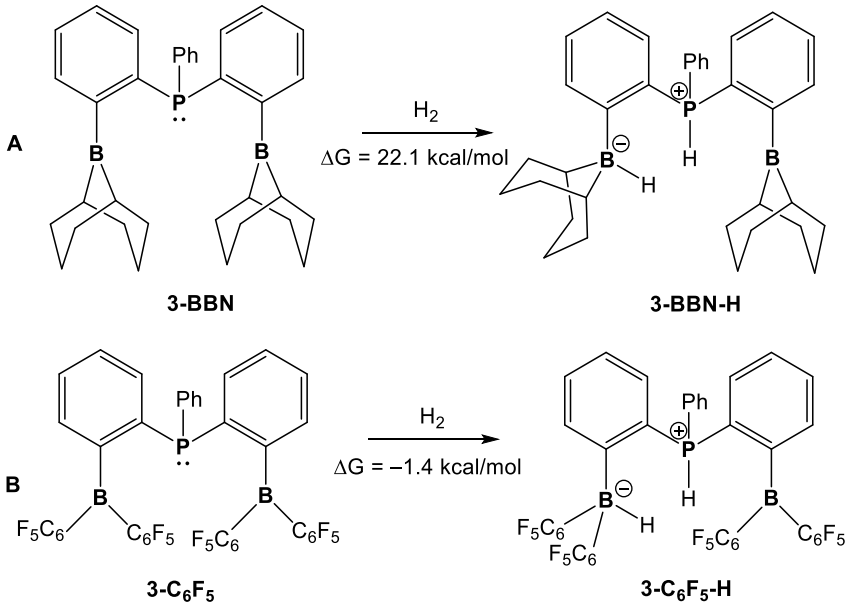
Figure 3-2. bisborane-phosphine FLP **3-BBN**.

In the next sections the reaction energies and reaction mechanism of the FLP **3-BBN** with small molecules (H_2, H_2O, CO, CN*t*Bu, MeOH) are presented.

3.1.1. Reaction with H_2

The activation of H_2 with FLP **3-BBN** was calculated to be thermodynamically unfavored (ΔG_{rxn} = 20.3 kcal/mol) and this is in line with the reported experimental observations of Dr. Rong Shang research group where no reaction was observed at ambient conditions.

Even though FLP **3-BBN** cannot activate H_2, if the boron center is substituted instead with the highly electron-withdrawing group $-C_6F_5$, the H_2 activation is favored (ΔG_{rxn} = −1.4 kcal/mol) with a plausible equilibrium displaced to the products (**Scheme 3-1**, **B**). Notoriously, the boranes in FLP **3-BBN** are weak Lewis acids.



Scheme 3-1. Reaction of FLP **3-BBN** and **3-C_6F_5** with H_2.

3.1.1. Reaction with H_2O

Almost all FLPs only activate HO–H bond (as shown in the Introduction section). But FLP **3-BBN** is one of the FLPs containing phosphorus and boron that reduces water at room temperature without the use of a transition metal.

According to the calculated reaction mechanism (**Figure 3-3**), a water molecule coordinates to one borane of **3-BBN** to give adduct **3-BH1** (ΔG_{R1} = −0.4 kcal/mol). Then the phosphine serves as a base to deprotonate the coordinated HO-H bond (via transition state **3-BTSH1**, $\Delta G_1^{\ddagger}$ = +7.7 kcal/mol) which generates intermediate **3-BH2** (ΔG_{R2} = −1.2 kcal/mol). The phosphonium cation now behaves as an electrophile to receive the pair of electrons of the

hydroxyl group while transferring the hydrogen as hydride to the second boron, **3-BTSH2** ($\Delta G_2^{\ddagger}$ = +14.5 kcal/mol) to form **3-BH3** (ΔG_{R3} = +8.6 kcal/mol). After that, a rotation of the B-C bond (**3-BTSH3**, $\Delta G_3^{\ddagger}$ = +1.0 kcal/mol) generates rotamer **3-BH4** (ΔG_{R4} = –2.5 kcal/mol) which keeps closer the hydrogens to finally lead to the formation of H_2 (via **3-BTSH4**, $\Delta G_4^{\ddagger}$ = +1.2 kcal/mol) and the phosphine oxide **3-BO** (ΔG_{R5} = –31.7 kcal/mol). Overall, the reaction is exergonic (ΔG°_R = –22.1 kcal/mol) with a total energy barrier of +18.0 kcal/mol. These calculations are in line with the reported observations of Dr. Rong Shang research group; they observe **3-BH2** by ^{1}H–NMR at -80°C.

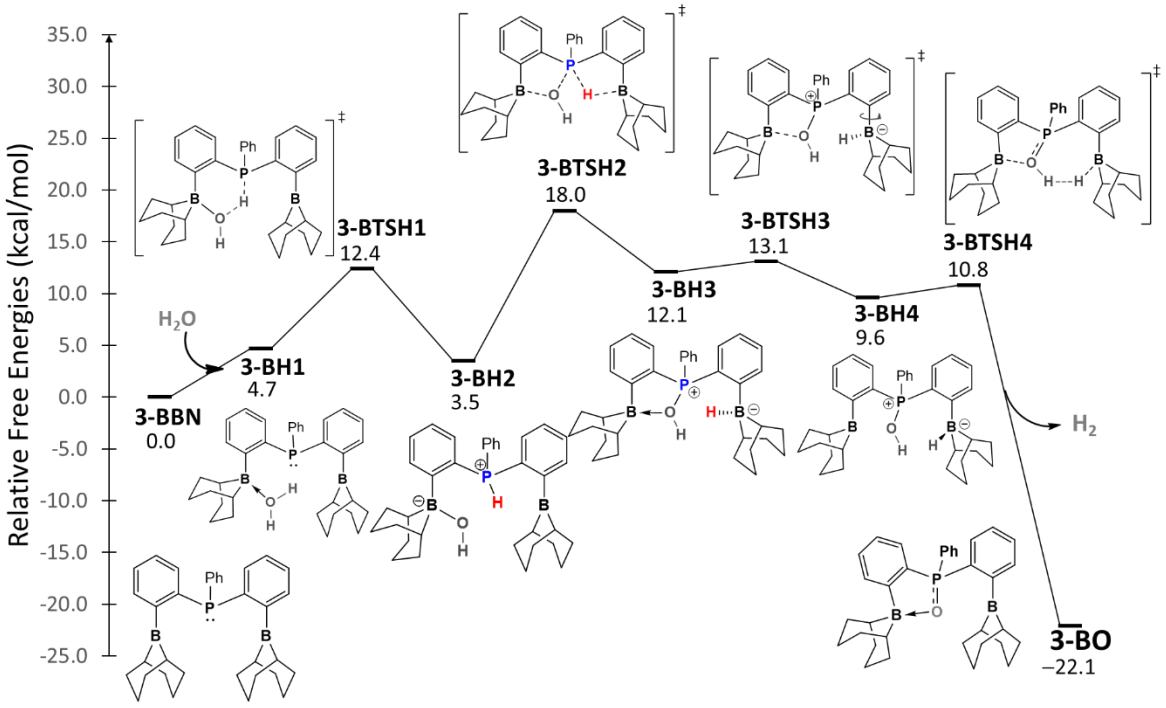


Figure 3-3. Proposed reaction mechanism of the water reduction with FLP **3-BBN**.

To further gain mechanistic insight of the reaction step from **3-BH2** to **3-BH3** an Intrinsic Reaction Coordinate (IRC) calculation was performed (**Figure 3-4**). Then for some structures, that are generated in the IRC output, a NBO charge calculation was executed (**Figure 3-4**,**B**). The NBO charges suggest that hydrogen of phosphine in **3-BH2** (**Figure 3-3**, **red hydrogen**) transforms into a hydride during the reaction step, as reflected in the charge change from positive to negative (**Figure 3-4**, **B**, **red line**), and the phosphine oxidizes; the charge becomes more positive (**Figure 3-4**, **B**, **blue line**). The hydrogen NBO charge has a minimum at the step 13 and the calculated IBOs of this reaction step reveals (**Figure 3-4**, **A**) that the hydride is not effectively bonded to boron and phosphorus, thus the charge accumulates at the hydride in this minimum.

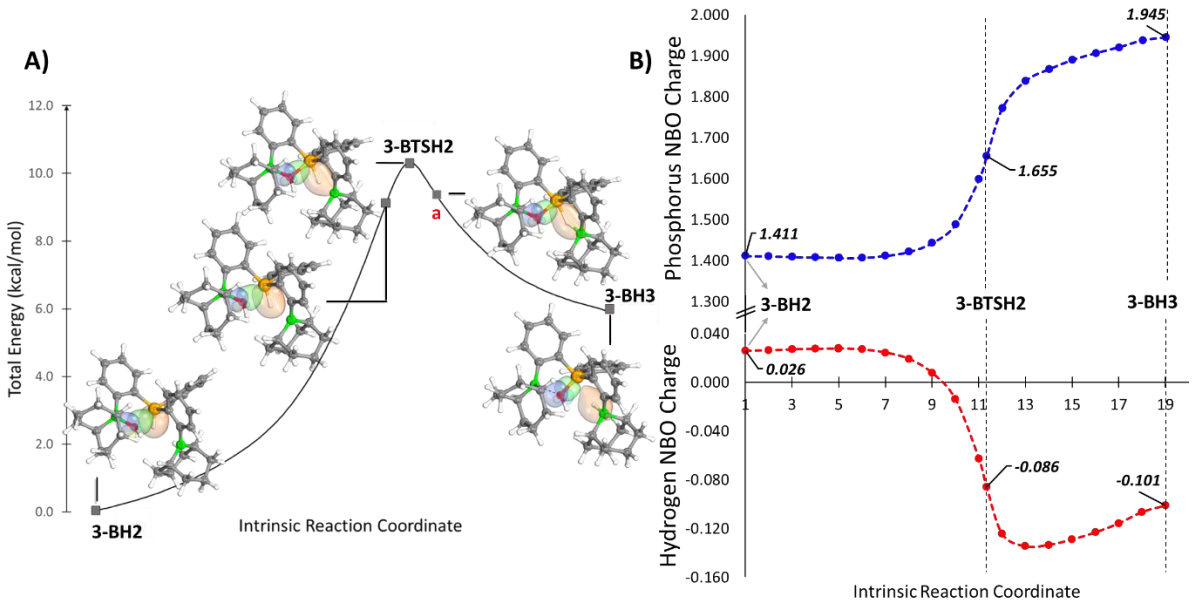


Figure 3-4. Generated Intrinsic Bond Orbitals (A) and NBO charges (B) of the IRC from **3-BH2** to **3-BH3**.

Moreover, a fluctional process was calculated for **3-BO** where the oxygen of phosphorus oxide migrates from boron to boron (**Figure 3-5**). As a first step, the oxygen decoordinates the borane of **3-BO** (via transition state **3-BTSH5**, $\Delta G_1^{\ddagger} = +8.4$ kcal/mol) generating rotamer **3-BOR** ($\Delta G_{R1} = 3.4$ kcal/mol). Then, a barrierless rotation of C–P bond proceeds to finally produce isomer **3-BOI** ($\Delta G_{R2} = -3.4$ kcal/mol). The low total energy barrier of +8.4 kcal/mol indicates a weak B–O coordination and this is in line with the experimental reports where only one ^{11}B NMR signal is observed of **3-BO**.

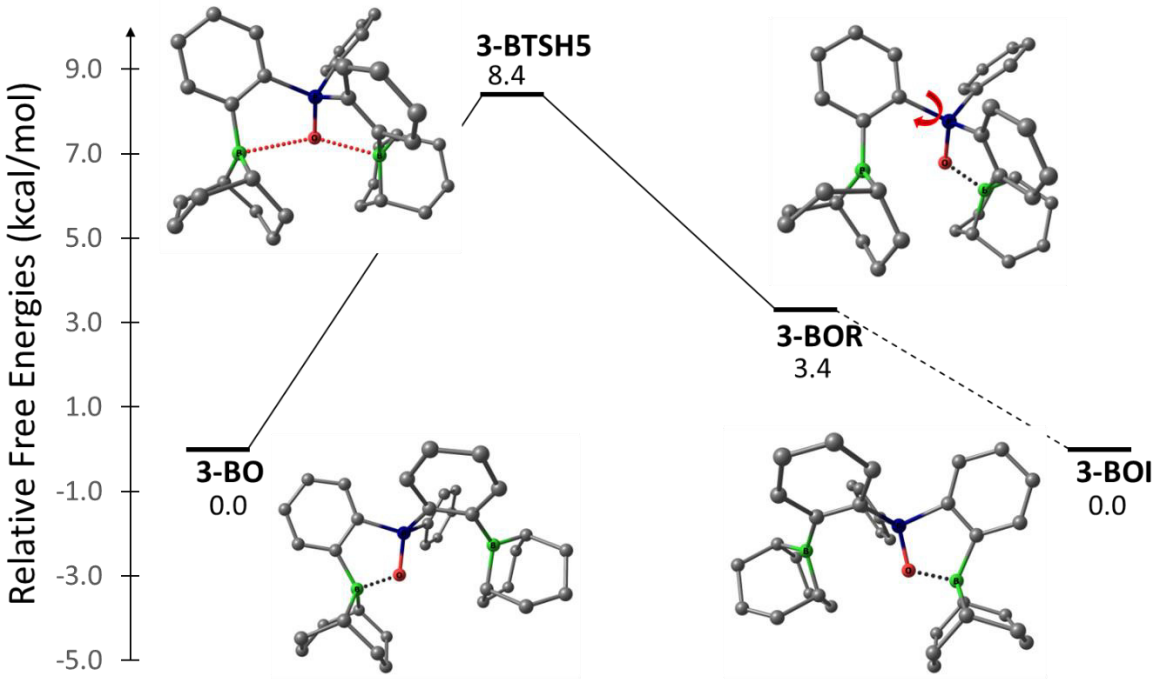


Figure 3-5. Calculated fluctional process of **3-BO**.

3.1.2. Reaction with MeOH and PhOH

As presented in the reduction of water with **3-BBN**, hydrogen and the phosphine oxide are produced **3-BO**. This led us to test computationally if the reduction could occur with MeOH to produce methane and **3-BO**. But unfortunately, the reduction has a high total energy barrier, and thus, does not proceed with FLP **3-BBN**.

To calculate the reaction mechanism, we took the optimized structures of **Figure 3-3** and changed the hydrogen of hydroxyl group for a methyl group (**Figure 3-6**). As a first step the coordination of methanol to one of the boranes of **3-BBN** occurs, generating adduct **3-BMe1** (ΔG_{R1} = –0.4 kcal/mol). Then, the phosphine deprotonates the hydrogen of hydroxyl (via transition state **3-BTSMe1**, $\Delta G_1^{\ddagger}$ = +6.5 kcal/mol) and produces **3-BMe2** (ΔG_{R2} = +4.1 kcal/mol). Later, the ethoxy group attacks the phosphine, transfering the hydrogen as hydride (**3-BTSMe2**, $\Delta G_2^{\ddagger}$ = +21.8 kcal/mol) to the second borane **3-BMe3** (ΔG_{R3} = +14.5 kcal/mol). After that, 3-BMe3 transforms into rotamer **3-BMe4** (ΔG_{R4} = +5.5 kcal/mol) which brings the methyl and the hydride closer to finally produce methane (**3-BTSMe3**, $\Delta G_3^{\ddagger}$ = +34.3 kcal/mol) and the phosphine oxide **3-BO** (ΔG_{R4} = –70.5 kcal/mol). Although this reaction is favored thermodynamically (ΔG°_R = –46.8 kcal/mol), it is kinetically not favored due to the high total energy barrier of 58.4 kcal/mol (practically unreachable). Experimentally **3-BMe2** is only observed by ^{1}H-NMR spectroscopy using a high excess of methanol. This is in line with the proposed reaction mechanism, where only the adduct **3-BMe1** and **3-BMe2** are accessible at room temperature and the reaction stops at this point because the following reaction steps are high in energy.

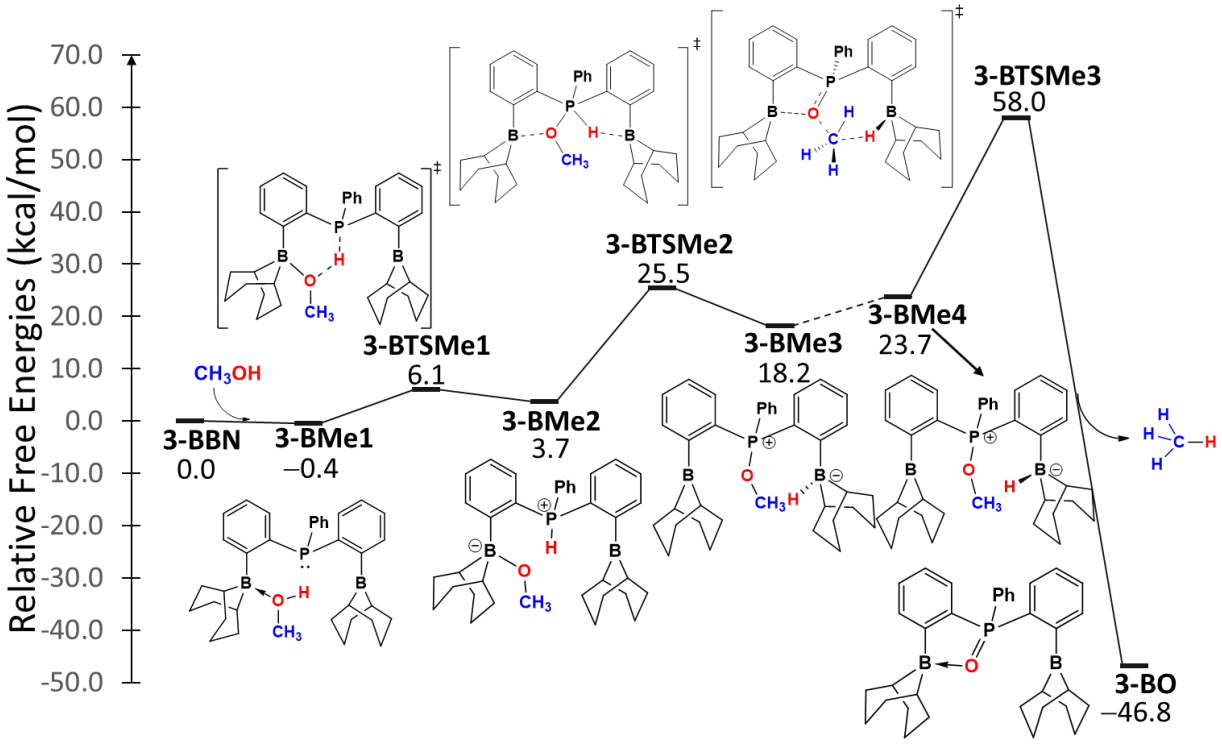


Figure 3-6. Calculated Energetic profile of the reaction of MeOH with FLP **3-BBN**.

Additionally, the energetic profile of the reaction of **3-BBN** with PhOH was also calculated (**Figure 3-7**). The results show the same trend as for the reaction with MeOH. The coordination of PhOH to one of the boranes of **3-BBN** is favored, generating **3-BPh1** (ΔG_{R1} = +3.4 kcal/mol). Then, the activation of O-H bond (ΔG_{R2} = –4.0 kcal/mol) is also plausible, leading to **3-BPh2**. However, attack of phenoxy group to phosphine is highly endergonic (ΔG_{R3} = –26.7 kcal/mol), the resulting intermediate **3-BPh3** is higher in energy than intermediate **3-BMe3** of the reaction of **3-BBN** with MeOH (**Figure 3-6**). The only difference between these intermediates is the bulkiness of the phenyl compared with the methyl group. Therefore, we attribute that intermediate **3-BPh3** is highly energetic due to steric repulsion of the phenyl group with the 9-borabicycloboryl groups (BBN).

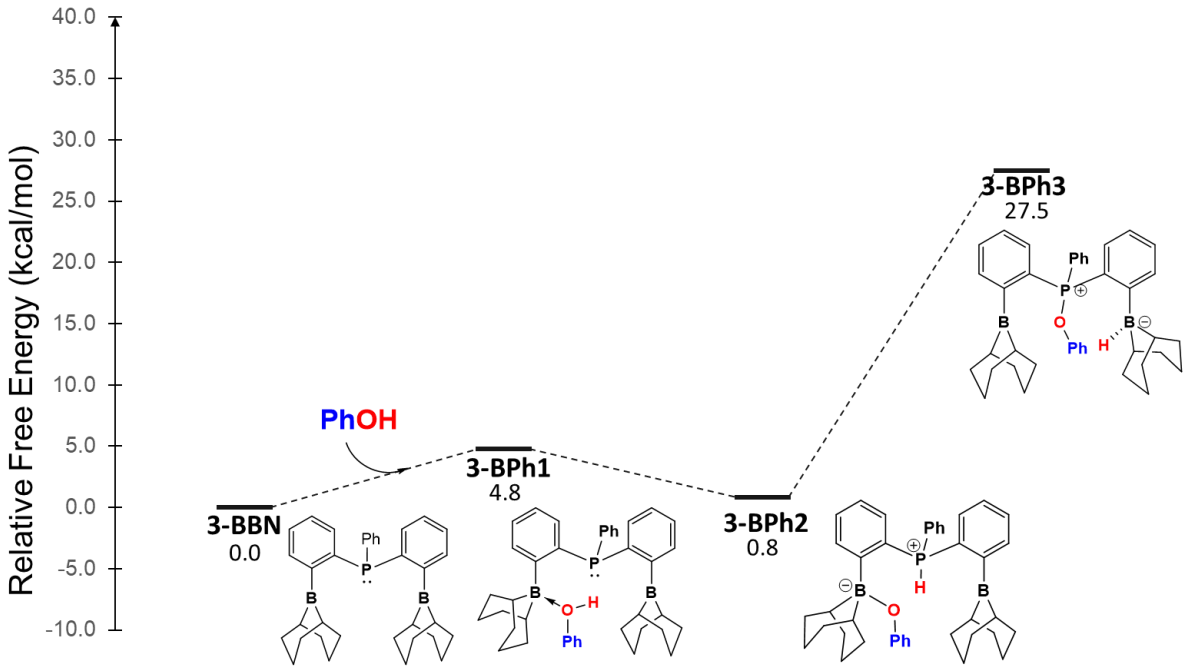


Figure 3-7. Calculated energetic profile of the reaction of **3-BBN** with PhOH.

3.1.3. Reaction with *n*BuSH

Knowing that the reaction of **3-BBN** with water produces H_2 and phosphine oxide, we proceeded to calculate the energetic profile of **3-BBN** with 1-butanethiol (**Figure 3-8**), used as an industrial solvent, to know if the thermodynamics favor the formation of phosphine sulfide **3-BS**, which is of great interest in many field of the chemistry.

According to the calculated energetic profile (**Figure 3-8**), the intermediates are high in energy compared with the reaction of **3-BBN** with water and methanol. Even though the overall reaction is exergonic ($\Delta G^{\circ}_R = -21.7$ kcal/mol), the highly energetic intermediate **3-BS3** with 31.7 kcal/mol (in relative free energies) does not favors the reaction to proceed.

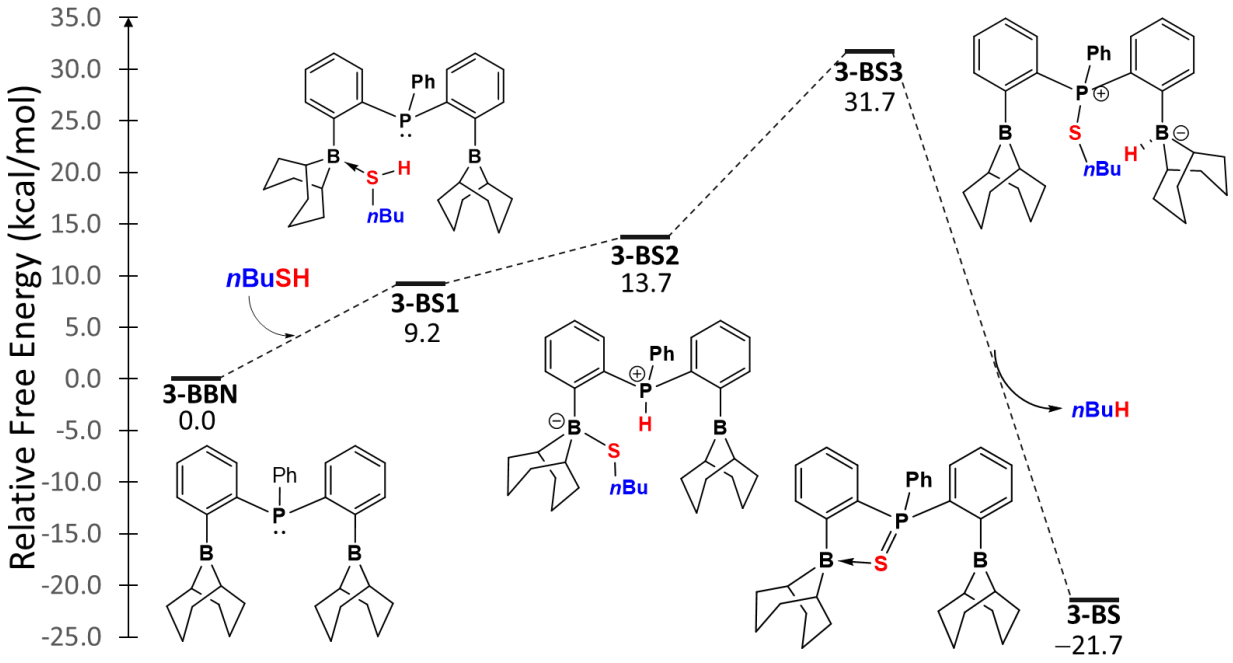


Figure 3-8. Calculated Energetic profile of the reaction of *n*BuSH with FLP **3-BBN**.

3.1.4. Reaction with CNtBu

In the reaction of **3-BBN** with CN*t*Bu, two equivalents of CN*t*Bu react with the two boranes of **3-BBN** to produce **3-BCN2**. The first coordination of one CN*t*Bu is favored and leads to **3-BCN1** (ΔG_{R1} = −5.9 kcal/mol). The second one produces **3-BCN2** (ΔG_{R1} = −1.6 kcal/mol) which, according to the calculations, is in equilibrium with intermediate **3-BCN1**. This equilibrium may be useful to make react borane **3-BCN1** with another nucleophilic molecule and further generate other type of products.

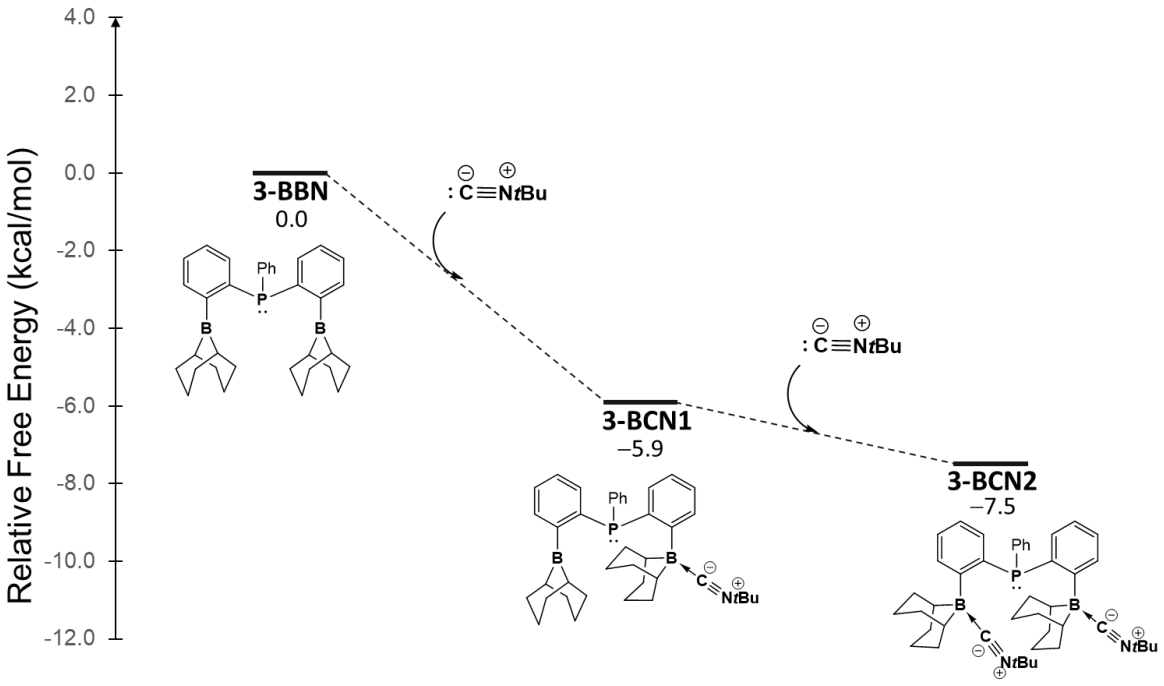


Figure 3-9. Calculated energetic profile of the reaction of 3-BBN with CN*t*Bu.

3.1.5. Reaction with CO

It is known that the frustrated Lewis pairs (FLPs) can fixate CO via a stepwise mechanism: the CO first coordinates the Lewis acid center and then, the Lewis base attacks carbon of CO (for further information see **CHAPTER 1**, **1.1.4**). The reaction generally stops at this point for most of the FLPs that contain boron and phosphorus. However, for **3-BBN** the reaction does not evolves to the expected product **3-BCl1**, instead leads to **3-BCO** (**Figure 3-10**).

The proposed reaction mechanism (**Figure 3-10**) starts first with the coordination of CO to one of the boranes of **3-BBN** leading to adduct **3-BCl1** (ΔG_{R1} = +3.0 kcal/mol). Then, phosphine attacks carbon of CO (**3-BCTS1**, $\Delta G_1^{\ddagger}$ = +3.0 kcal/mol) generating intermediate **3-BCl2** (ΔG_{R2} = +1.3 kcal/mol). Generally, the fixation of CO stops at this point for most of FLPs but the existence of the second borane makes that oxygen of the carbonyl of **3-BCl2** coordinates this borane (**3-BCTS2**, $\Delta G_2^{\ddagger}$ = +6.1 kcal/mol) producing **3-BCl3** (ΔG_{R3} = +0.7 kcal/mol). Carbonyl carbon of **3-BCl3** is highly acidity, hence the carbon migration of the 9-borabicyclononane (BBN) occurs slowly (**3-BCTS3**, $\Delta G_3^{\ddagger}$ = +13.7 kcal/mol), leading to exergonic intermediate **3-BCl4** (ΔG_{R4} = –8.6 kcal/mol). Finally, oxygen bonds to the second borane (**3-BCTS4**, $\Delta G_4^{\ddagger}$ = +1.4 kcal/mol) generating product **3-BCO** (ΔG_{R5} = –4.1 kcal/mol). The overall barrier (18.7 kcal/mol) and reaction (ΔG° = –20.0 kcal/mol) energy agree with the experimental information: the reaction is done at room temperature.

Moreover, two entropy corrections were applied to this reaction mechanism. If this was not done the free energy barrier would be 22.17 kcal/mol which is inconsistent with the enthalpy energy barrier of 12.4 kcal/mol. This high difference indicates that the entropy is not calculated correctly. Therefore, we applied Grimme's Quasi Rigid Rotor Harmonic approximation which is

an interpolation between harmonic and free-rotor approximation as implemented in Shermo program.[72] Also, the energetic profile was calculated at the pressure of 274 atm to simulate the solvent effect of benzene.

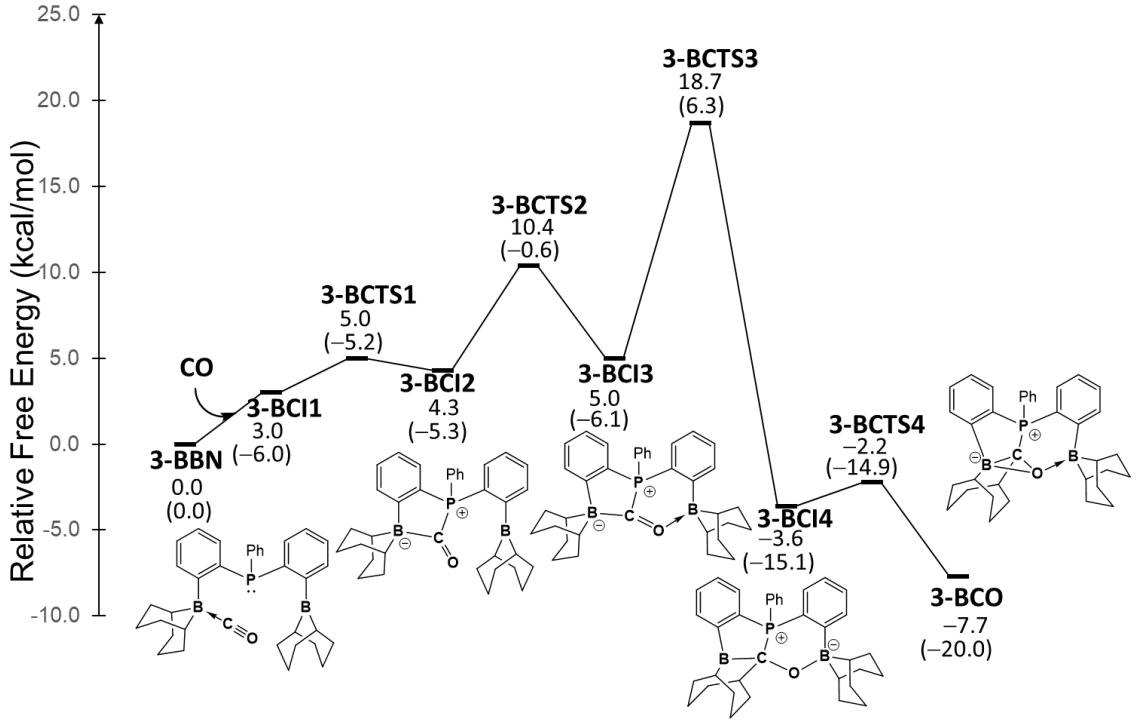


Figure 3-10. Proposed reaction mechanism of **3-BBN** with CO (P = 274 atm). Numbers in parenthesis are in enthalpy scale.

3.2. Bisborane-Phosphine BPB 3-Cy

Changing the substituents of boron of **3-BBN** by cyclohexyls (**3-Cy**) (**Figure 3-11**) confers a different reactivity of **3-Cy** with H_2O and CO. This can be attributed to the fact that migration of a cyclohexyl of **3-Cy** is more feasible than boron substituents in **3-BBN**.

Reaction of **3-Cy** with H_2O and CO have the same by–product; a tricyclohexylborane. Experimentally, the evidence of this by–product is its crystal structure. However, the structure of the main product is proposed by NMR. Moreover, it is proposed that **3-Cy** is in equilibrium with the free tricyclohexylborane and the proposed intermediate **3-CyPB**. This could explain why in the reaction of **3-Cy** with H_2O and CO the tricyclohexylborane is observed.

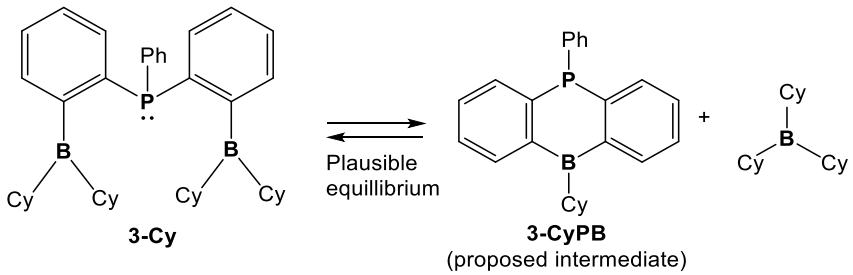


Figure 3-11. bisborane–phosphine FLP **3-Cy** proposed equilibrium with **3-CyPB**.

According to quantum mechanical calculations, conversion of **3-Cy** to **3-CyPB** is thermodynamically favored, and the reaction energy of ΔG_{Rxn} = –5.4 kcal/mol indicates that **3-CyPB** would be mainly observed experimentally. Furthermore, different reaction paths are proposed for this conversion (**Figure 3-12**). The first reaction path (**Figure 3-12**, black line) involves a highly endergonic intermediate **3-CyI1** (ΔG_{1Black} = 60.2 kcal/mol). The second reaction path (**Figure 3-12**, blue line) contains an accessible intermediate, **3-CyI2**, at room temperature (ΔG_{1Blue} = 11.9 kcal/mol). Two transition states are proposed that can lead to this intermediate. In both, the phenyl moiety of the phosphine migrates towards the second borane. Migration of the ipso (**3-CyTS1**, $\Delta G_1^{\ddagger}$ = +63.5 kcal/mol) and ortho (**3-CyTS2**, $\Delta G_{1\_2}^{\ddagger}$ = +45.0 kcal/mol) carbon towards the second borane are both highly endergonic, thus, intermediate **3-CyI2** is not accessible at room temperature. Other transition states could be proposed that could lead to intermediate **3-CyI1**, however, the final step to generate **3-CyPB** and the tricyclohexylborane through transition state **3-CyTS3** is also highly endergonic ($\Delta G_2^{\ddagger}$ =40.4 kcal/mol). Overall, even though conversion of **3-Cy** to **3-CyPB** is thermodynamically favored, kinetically is not favored.

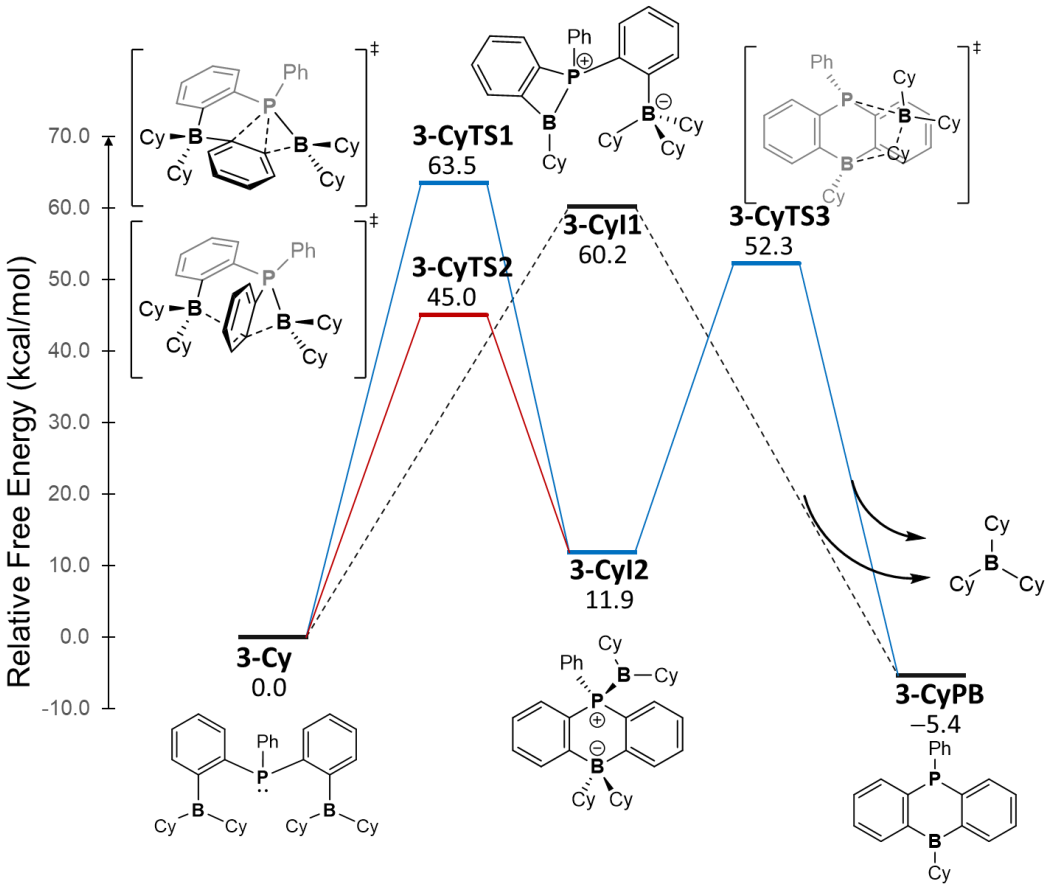
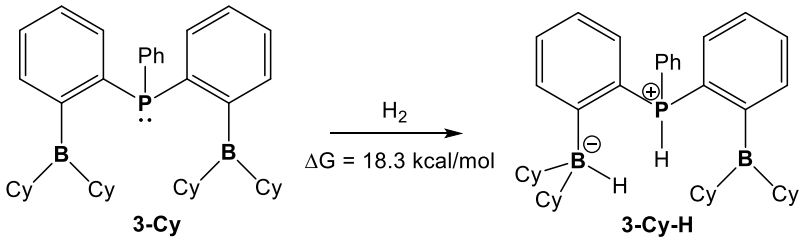


Figure 3-12. Proposed reaction paths for the conversion of **3-Cy** to **3-CyPB**.

3.2.1. Reaction with H_2

Reaction of **3-Cy** with H_2 is slightly less endergonic (ΔG_{Rxn} = 18.3 kcal/mol) (**Scheme 3-2**) compared with its analog **3-BBN** (ΔG_{Rxn} = 22.1 kcal/mol) (**Scheme 3-1**). This is also an indicator that boranes in **3-Cy** are more acidity than the ones in **3-BBN**. Though reaction of **3-Cy** with H_2 is less endergonic, the reaction energy is still high, therefore the activation of H_2 is not favored even with heating.



Scheme 3-2. Reaction of **3-Cy** with H_2.

3.2.2. Reaction with H_2O

For the reaction of **3-Cy** with water (**Figure 3-13**), we first took as model the previously shown reaction mechanism of **3-BBN** with water. The reaction starts first with the coordination of water with one of the boranes of **3-Cy** leading to adduct **3-CH1** (ΔG_1 = +0.9 kcal/mol). Then, deprotonation occurs via transition state **3-CTSH1** ($\Delta G_1^{\ddagger}$ = +3.4 kcal/mol) generating intermediate **3-CH2** (ΔG_2 = +0.3 kcal/mol). This reaction step has a lower energy barrier than the analogous reaction step shown for FLP **3-BBN** (**Figure 3-3**, **3-BTSH1**, $\Delta G_1^{BBN\ddagger}$ = +7.7 kcal/mol). After that, hydroxyl group of borane attacks phosphorus atom and displaces the hydrogen as hydride towards the second borane (**3-CTSH2**, $\Delta G_2^{\ddagger}$ = +15.2 kcal/mol), producing intermediate **3-CH3** (ΔG_3 = +4.1 kcal/mol). The following reaction step is barrierless and corresponds to the attack of hydride of borane towards the proton of hydroxyl phosphine, producing the phosphine oxide **3-CyO** (ΔG_4 = –27.3 kcal/mol). A second water attacks the free borane and leads to the exergonic intermediate **3-CyOH** (ΔG_5 = –3.0 kcal/mol). The main differences of this reaction mechanism compared to the one calculated for FLP **3-BBN** is that the overall energy barrier for FLP **3-Cy** is +16.4 kcal/mol, which is lower than the one calculated for FLP **3-BBN** (+18.0 kcal/mol) and the overall intermediate and transition states energies of **3-Cy** are much lower than the ones calculated for **3-BBN**. This shows that **3-Cy** is more reactive than **3-BBN**, attributed to the boranes in **3-Cy** which are whose acidity is larger than boranes in **3-BBN**.

As already mentioned, one of the reaction products of **3-Cy** with H_2O is tricyclohexylborane and other product that does not corresponds to **3-BCO** or **3-BCOH**. Therefore, the reaction may proceed through other reaction mechanism or by not stopping at intermediate **3-BCOH** and continuing to other product. However, the calculated energetic profile in **Figure 3-13** shows that FLP **3-Cy** is more reactive than **3-BBN**.

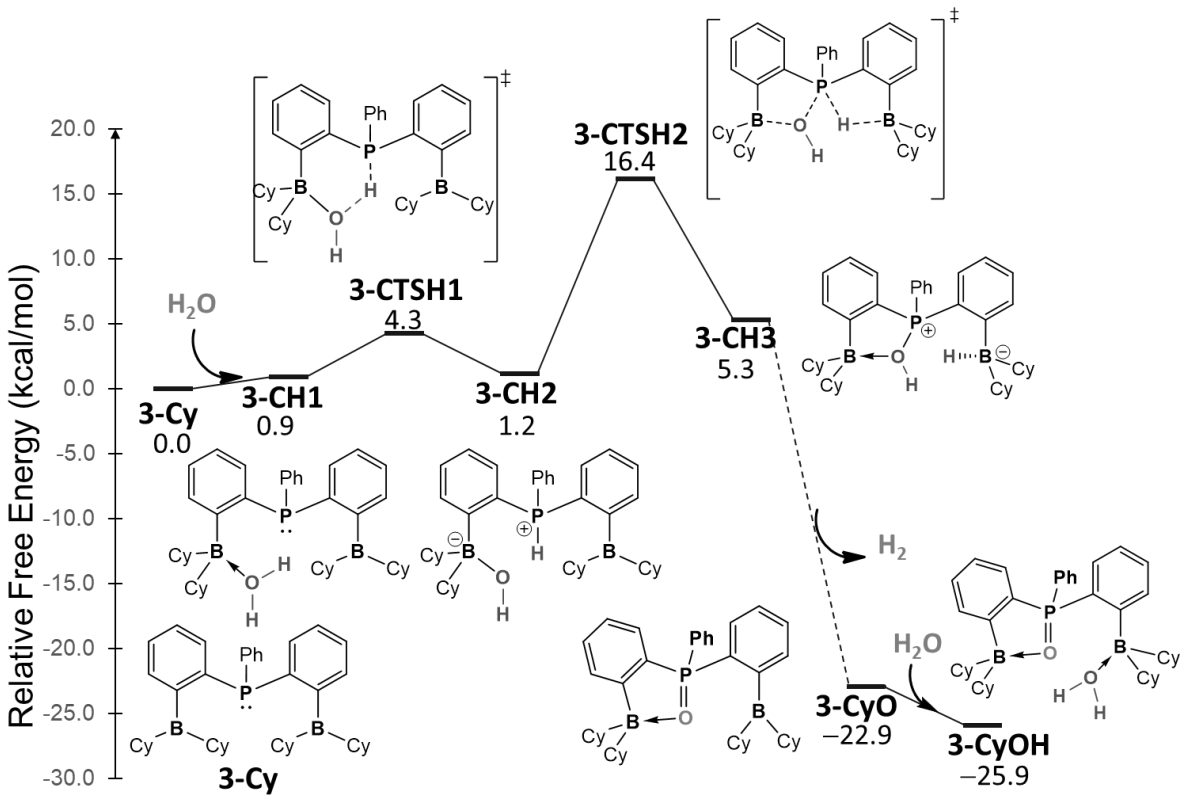


Figure 3-13. Reaction mechanism of **3-Cy** with water, as it was proposed for FLP **3-BBN**.

3.2.3. Reaction with CO

The previously calculated reaction mechanism of **3-BBN** with CO was also used to understand how the reaction may proceed but now with FLP **3-Cy**. Only relevant reaction steps were calculated for this reaction mechanism (**Figure 3-14**). First, the coordination of CO with a borane of **3-Cy** generates adduct **3-CCI1** (ΔG_1 = +3.2 kcal/mol). After a few reaction steps, intermediate **3-CCI2** is produced (ΔG_1 = +2.4 kcal/mol). Migration of cyclohexyl proceeds via transition state **3-CCTS1** ($\Delta G_1^{\ddagger}$ = +11.4 kcal/mol), leading to intermediate **3-CCI3** (ΔG_2 = –6.9 kcal/mol). Finally, a ring closure occurs and generates structure **3-CCO** (ΔG_2 = –8.4 kcal/mol). The total energy barrier of this reaction mechanism is 13.8 kcal/mol, which is even lower than the one calculated for FLP **3-BBN** (18.7 kcal/mol). This is attributed to the facility of cyclohexyl to migrate over the borane substituents of **3-BBN**.

Even though, this reaction mechanism is favored due to the low total energy barrier, more investigations need to be done because two products are mainly observed, one of them corresponds to the tricyclohexylborane. This indicates that the reaction does not concludes in **3-CCO** and continues to other product.

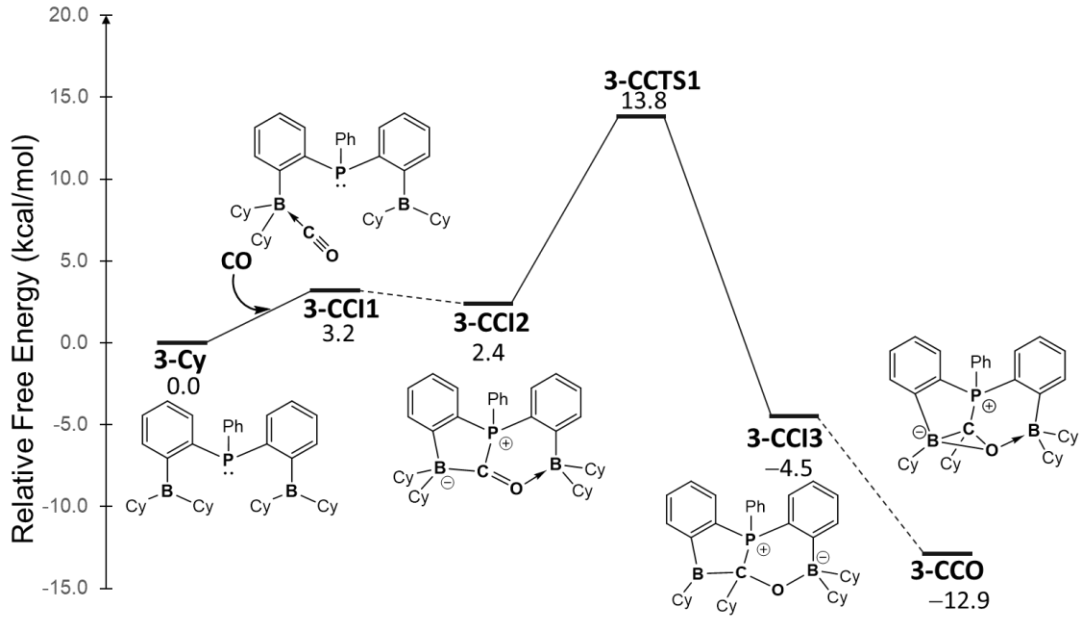
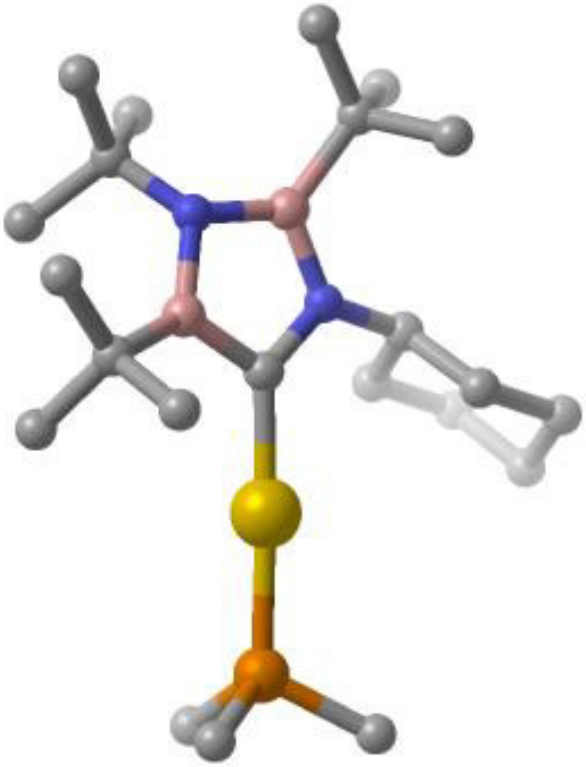


Figure 3-14. Reaction mechanism of **3-Cy** with CO, as it was proposed for FLP **3-BBN**.

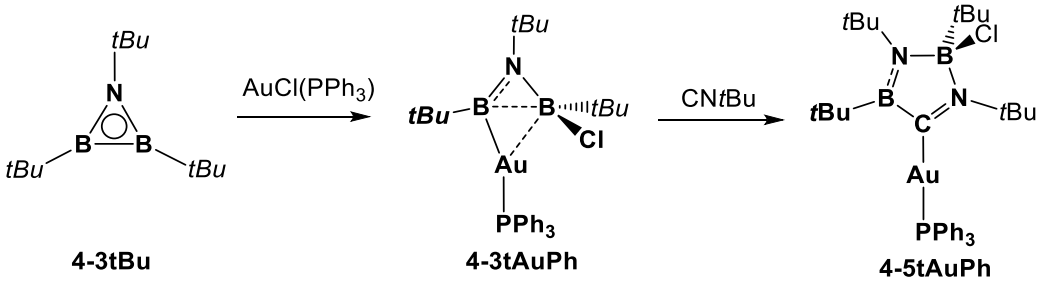
CHAPTER 4



In this chapter, first the energetic profile for the reaction of three different azadiboriridine derivatives (Mesityl, *diiso*-propyl and *tert*-Butyl substituted) with gold(I) complexes is presented. Then, the reaction mechanism of these complexes with isocyanide *t*BuNC to produce the BNC carbene gold(I) complexes is shown. After that, the electronic structure of the latter complex and its reduce form is studied by means of theories of Intrinsic Bond Orbitals (IBO), Natural Bond Orbitals (NBO) and Molecular Orbitals (MO). Finally, the π–accepting and σ–donating properties of these new BNC gold(I) complexes is compared among the CAAC and NHC gold(I) complexes. All the experimental data was provided by Dr. Rong Shang's student, Yoshitaka Kimura from the University of Hiroshima.

4.1. Azadiboriridine gold(I) complexes

Recently, it was reported by Dr. Rong Shang research group that azadiboriridine **4-3tBu** reacts with various gold(I) complexes to produce azadiboriridine gold(I) complexes **4-3tAuPh** (**Figure 4-1**).[73] The later complexes can be reacted with an isocyanide (CN*t*Bu) to afford **4-5tAuPh**. For the first time, these reactions develop a methodology to synthesize BNC gold(I) carbenes complexes.



4-3tBu **4-3tAuPh** **4-5tAuPh**

Figure 4-1. Reaction of azadiboriridine **4-3tBu** with AuCl(PPh_3) and CN*t*Bu.

4.1.1. Mesityl derivative

The reaction shown in **Figure 4-1** can be further developed for azadiboriridines with a mesityl substituent in one boron atom and in the other boron the tertbutyl substituent remains. Two main differences can be found for the –*t*Bu and –Mes derivatives: 1) phosphines always coordinate gold atom for the –Mes derivatives while strong phosphines or ligands (such as 4-dimethylaminopyridine (DMAP)) coordinate boron atom of the –*t*Bu derivatives (**Figure 4-2**). 2) The most exergonic complex of the –Mes derivates is the one substituted with PCy_3 (**Figure 4-4**, **4-3MAuCy**) and for –tBu derivatives is the complex that contains the DMAP ligand[73] (**Figure 4-3**). These differences are mainly attributed to the mesityl group which is bulkier than *t*Bu, thus the steric hindrance between mesityl and phosphines leads to favor the coordination of phosphines into gold atom.

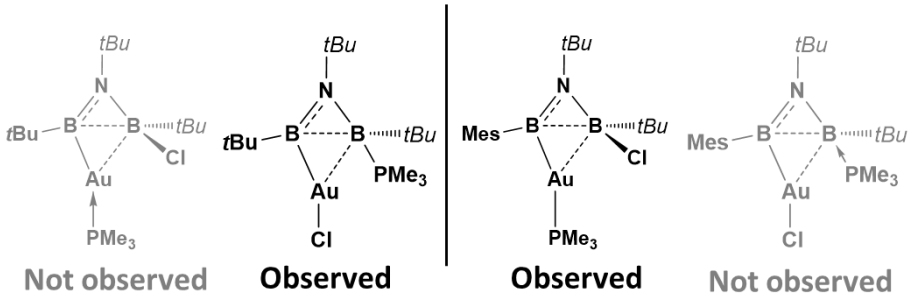


Figure 4-2. The most thermodynamically stable isomer of the –tBu and –Mes azadiboriridine gold(I) complexes with PMe_3 as ligand.

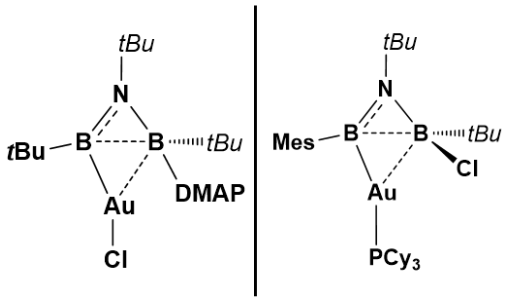


Figure 4-3. Most exergonic complex of the –tBu and –Mes azadiboriridine gold(I) complexes.

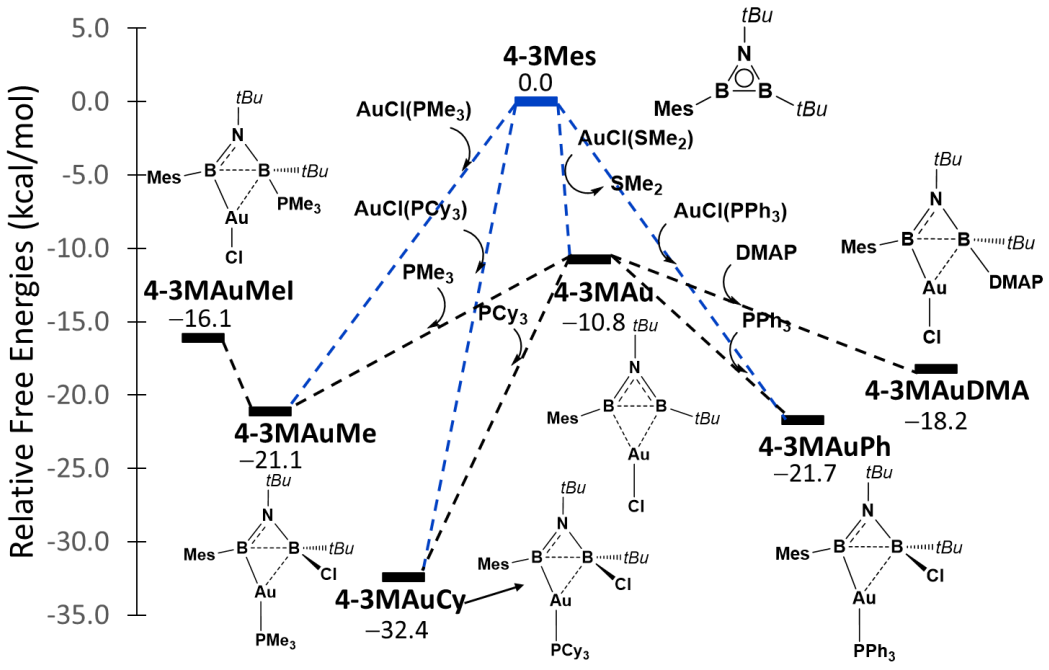


Figure 4-4. Calculated energetic profile for the formation of the gold azadiboriridine gold(I) complexes.

4.1.2. Diisopropylamino derivative

An interesting property of the azadiboriridine diisopropylamino derivative (**4-3NiPr**) is that the substituted diisopropylamino group in the boron atom and the nitrogen of the three-membered ring are stabilizing the boron vacant *p*-orbital. Therefore, a total of two electron pairs stabilizes the boron *p*-orbital. On the other hand, the tertbutyl and mesityl derivatives only have one nitrogen that stabilizes boron *p*-orbital. The calculated Molecular Orbitals (MO) of **4-3NiPr** corroborate this proposal (**Figure 4-5**), where **HOMO-1** shows a π(N-B) bond from the diisopropylamino fragment to the boron and **HOMO-3** shows a conjugation of the nitrogen electron pair of diisopropylamino substituent to the π-cloud of the three-membered ring.

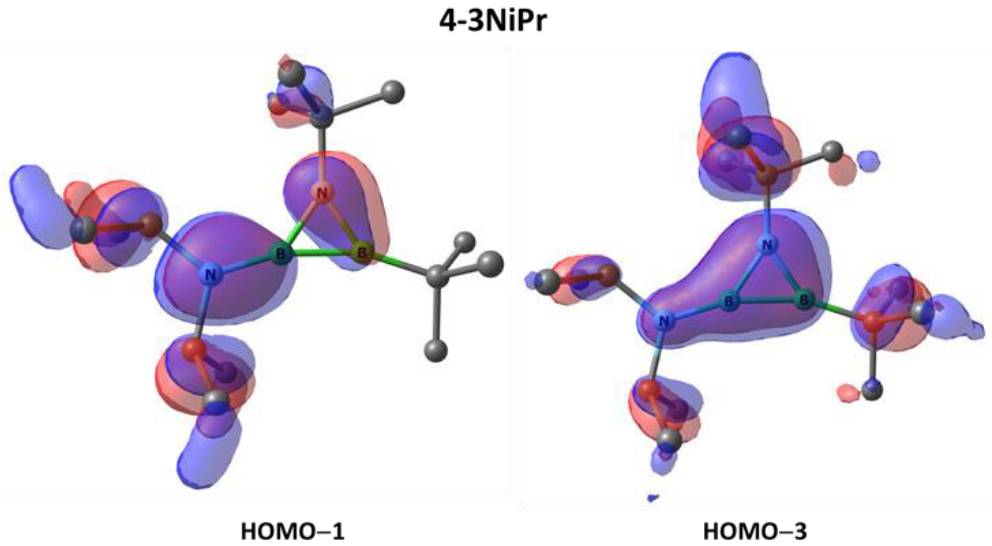


Figure 4-5. Relevant Molecular Orbitals of the azadiboriridine diisopropylamino derivative **4-3NiPr**. Isosurface = 0.03 a.u.

The previously mention electronic structure difference of the azadiboriridine diisopropylamino derivative (**4-3NiPr**) from the –Mes (**4-3Mes**) and –*t*Bu (**4-3tBu**) derivatives, leads to **4-3NiPr** containing a different reactivity. The reaction of **4-3NiPr** with AuCl(PCy$_3$) do not forms an azadiboriridine gold(I) complex as shown for –tBu and –Mes azadiboriridines derivatives (**Figure 4-1**, **Figure 4-4**), instead complex **4-3NAuCy** is generated (**Figure 4-6**). The proposed reaction mechanism (**Figure 4-6**) starts with the cleavage of B–B bond of **4-3NiPr** by AuCl(PCy$_3$) (via transition state **4-3NTS1**, $\Delta G_1^{\ddagger}$ = +12.0 kcal/mol) to generate **4-3NI1** (ΔG_{R1} = +1.8 kcal/mol). Then, chloride migrates towards the boron substituted with a tert-butyl (**4-3NTS2,** $\Delta G_2^{\ddagger}$ = +3.6 kcal/mol) and produces **4-3NI2** (ΔG_{R2} = –6.0 kcal/mol) which was the expected product of Dr. Rong Shang's research group. Finally, the borane decoordinates from gold atom (**4-3NTS3,** $\Delta G_2^{\ddagger}$ = +3.9 kcal/mol) producing **4-3NAuCy** (ΔG_{R3} = –5.5 kcal/mol). The final step is favored due to the formation of a π bond between each nitrogen and boron atoms in

4-3NAuCy. Overall, the reaction is exergonic (ΔG°_{R} = –9.7 kcal/mol) with a total energy barrier of 12.0 kcal/mol which is controversy with the experiment; heating the reaction to 50°C is needed to proceed. We expect a hidden low energy intermediate that may generate and thus increases the total barrier energy.

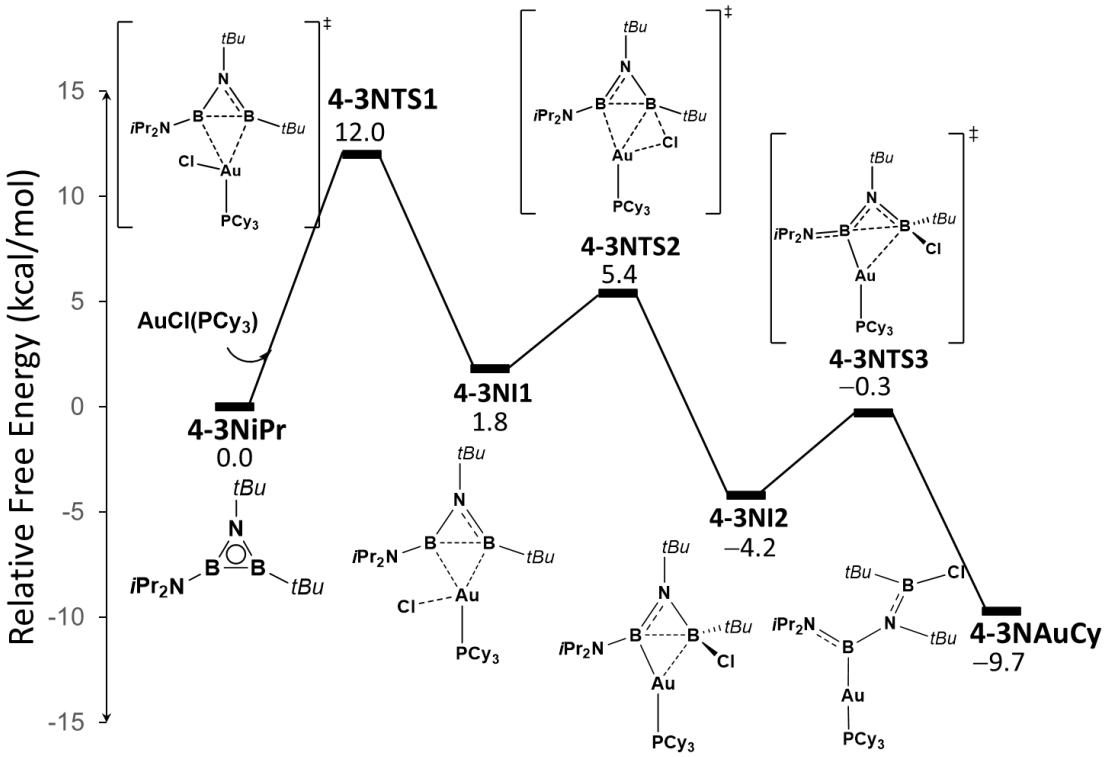
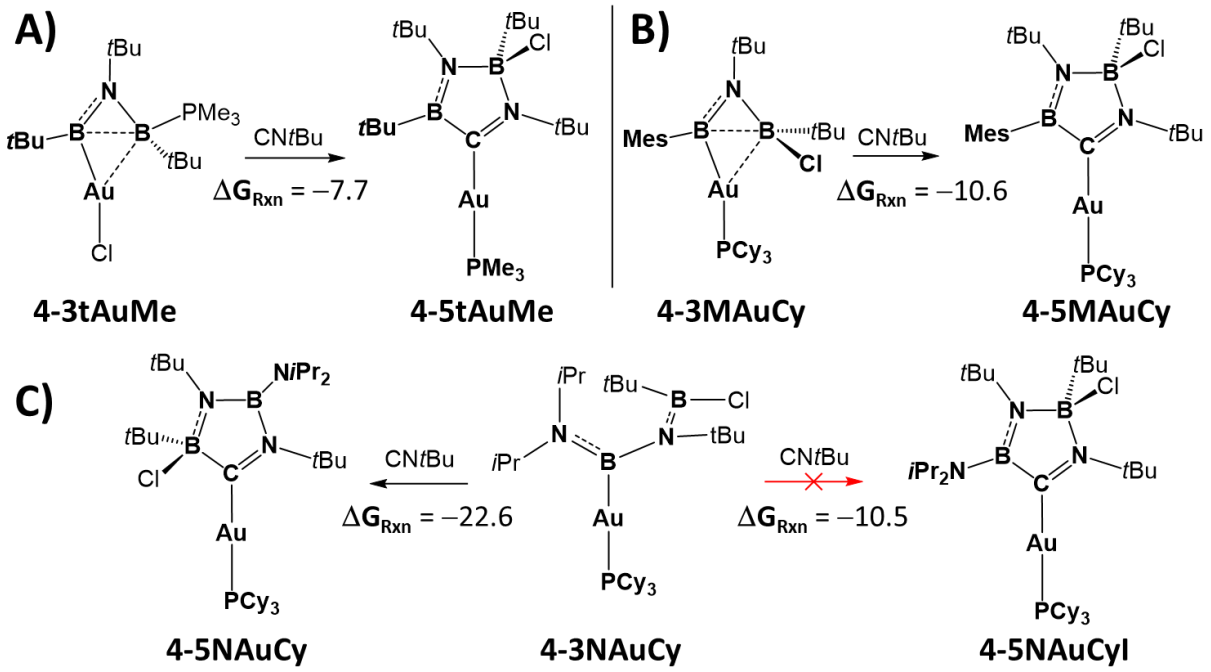


Figure 4-6. Proposed reaction mechanism of **4-NiPr** with AuCl(PCy_3).

4.2. Formation of BNC gold(I) complexes

As I already mentioned, –*t*Bu azadiboriridine gold(I) complexes can react with CN*t*Bu to form BNC gold(I) complexes (**Scheme 4-1**, **A**). It is expected that the –Mes and –$NiPr_2$ gold(I) derivatives can also form these complexes. Indeed, in **Scheme 4-1** the calculated reaction energies for the –Mes (**B**, ΔG_{Rxn} = –10.6 kcal/mol) and –$NiPr_2$ (**C**, ΔG_{Rxn} = –22.6 kcal/mol) gold(I) derivatives show that the thermodynamics are favored for the formation of BNC gold(I) complex. However, –$NiPr_2$ gold(I) derivative does not forms the expected product **4-5NAuCyI**, instead **4-5NAuCy** is observed experimentally and this is in line with the calculated reaction energies. Therefore, the reaction mechanism of –$NiPr_2$ gold(I) derivative (**4-3NAuCy**) with CN*t*Bu is different than for the –tBu (**4-3tAuMe**) and –Mes (**4-3MAuCy**) gold(I) derivatives.



Scheme 4-1. Calculated reaction free energies of the reactions of azadiboriridine gold(I) complexes with CN*t*Bu.

4.2.1. Tert-butyl Derivative

It was already reported[73] in our group a computed reaction mechanism of a –*t*Bu azadiboriridine gold(I) complex with *t*BuNC. In the studied system the phosphine is bonded to gold atom (for example, see **4-3tAuPh** from **Figure 4-1**). However, the reaction mechanism for the –*t*Bu gold(I) derivative **4-3tAuMe** (**Scheme 4-1**) which has a phosphine bonded to a borane was not considered yet. Thus, we proceeded to calculate the reaction mechanism of **4-3tAuMe** with *t*BuNC (**Figure 4-7**). First, the isocyanide *t*BuNC coordinates the free borane (**4-3tTS1**, $\Delta G_1^{\ddagger}$ = +15.9 kcal/mol) leading to adduct **4-3tI1** (ΔG_{R1} = +11.8 kcal/mol). After that, the phosphine decoordinates borane (**4-3tTS2**, $\Delta G_2^{\ddagger}$ = +0.1 kcal/mol) generating **4-3tI2** (ΔG_{R2} = –11.7 kcal/mol). Then, phosphine coordinates but towards the gold atom (**4-3tTS3,** $\Delta G_3^{\ddagger}$ = +12.3 kcal/mol) producing **4-3tI3** (ΔG_{R3} = +3.1 kcal/mol). Barrierless isomerization of **4-3tI4** generates **4-3tI5** (ΔG_{R4} = +3.2 kcal/mol) which brings closer the chloride to the free borane so it can migrate (**4-3tTS4,** $\Delta G_4^{\ddagger}$ = +5.7 kcal/mol) making **4-3tI5** (ΔG_{R5} = +1.2 kcal/mol). Now, gold atom migrates towards the carbon of the isocyanide (**4-3tTS5,** $\Delta G_4^{\ddagger}$ = +3.6 kcal/mol) leading to **4-3tI6** (ΔG_{R6} = –2.9 kcal/mol). Finally, the cyclization occurs (**4-3tTS6,** $\Delta G_5^{\ddagger}$ = +5.4 kcal/mol) and generates the expected BNC gold(I) complex **4-5tAuMe** (ΔG_{R6} = –12.5 kcal/mol). Overall, the reaction is thermodynamically favored with a reaction free energy of ΔG°_R = –9.7 kcal/mol. Experimentally, the reaction occurs at room temperature and agrees with the calculated total barrier energy of 15.9 kcal/mol.

The reaction mechanism of the –Mes azadiboriridine gold(I) complexes (**Scheme 4-1**, **B**) with *t*BuNC are expected to follow a similar reaction mechanism to the –*t*Bu gold(I) derivatives

(**Scheme 4-1**, **A**) proposed initially in our group.[73] Therefore, that energetic profile was not calculated.

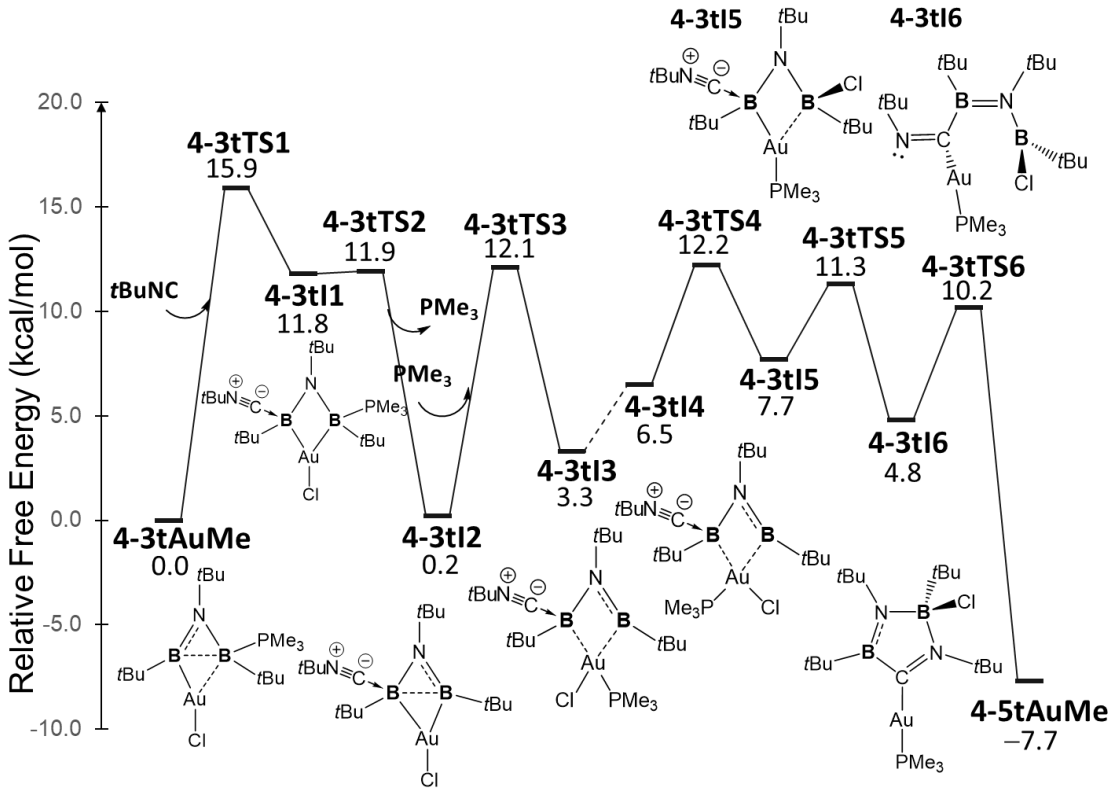


Figure 4-7. Plausible reaction mechanism of −*t*Bu azadiboriridine gold(I) complex (**4-3tAuMe**) with *t*BuNC.

4.2.2. Diisopropylamino derivative

The −N*i*Pr$_2$ gold(I) derivative (**4-3NAuCy**) contains two different Lewis acids that can interact with CyNC (**Figure 4-8**). To know which boron is more plausible to be attacked, the energetic profile of the addition of CyNC to **4-3NAuCy** was calculated (**Figure 4-9**). It revealed that the boron bonded to gold is less plausible to be attacked due to the calculated high barrier energies (**Figure 4-9**, red lines). Two different transition states are computed for this attack, both are early transition states. In one of them, CyNC coordinates to the outer part of boron (**4-3B1OTS**) and has a barrier energy of 32.9 kcal/mol and, in the other, CyNC coordinates to the inner part of boron (**4-3B1iTS**) and has barrier energy of 25.5 kcal/mol. On the other hand, the attack of CyNC towards the boron bonded to chloride is plausible (**Figure 4-9**, black lines), the calculated energy barriers for the attack of CyNC at the inner (**4-3B2CliTS**) and outer (**4-3B2ClOTS**) part of this boron atom are of 20.2 kcal/mol and 18.4 kcal/mol, respectively. However, the addition of CyNC to the inner part of boron (**4-3B2CliTS**) is not favored because it generates highly energetic intermediates such as **4-3NAI1a** that has a free relative energy of

21.2 kcal/mol. Therefore, the addition of CyNC to the outer part of boron bonded to chloride (**4-3B2ClOTS**) is the preferred route of this reaction mechanism.

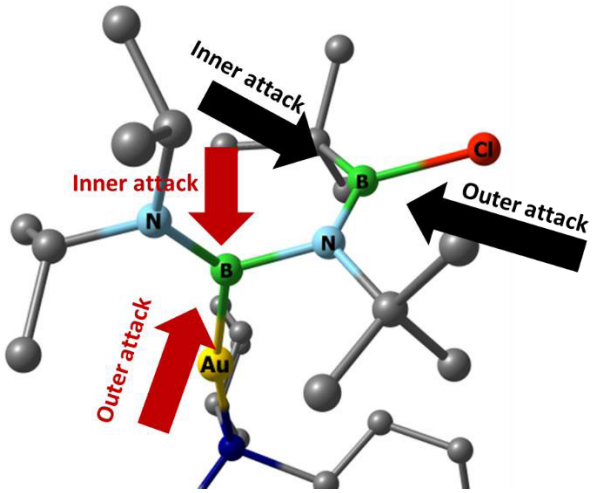


Figure 4-8. Lewis acids sites and the orientations in **4-3NAuCy** where CyNC can attack.

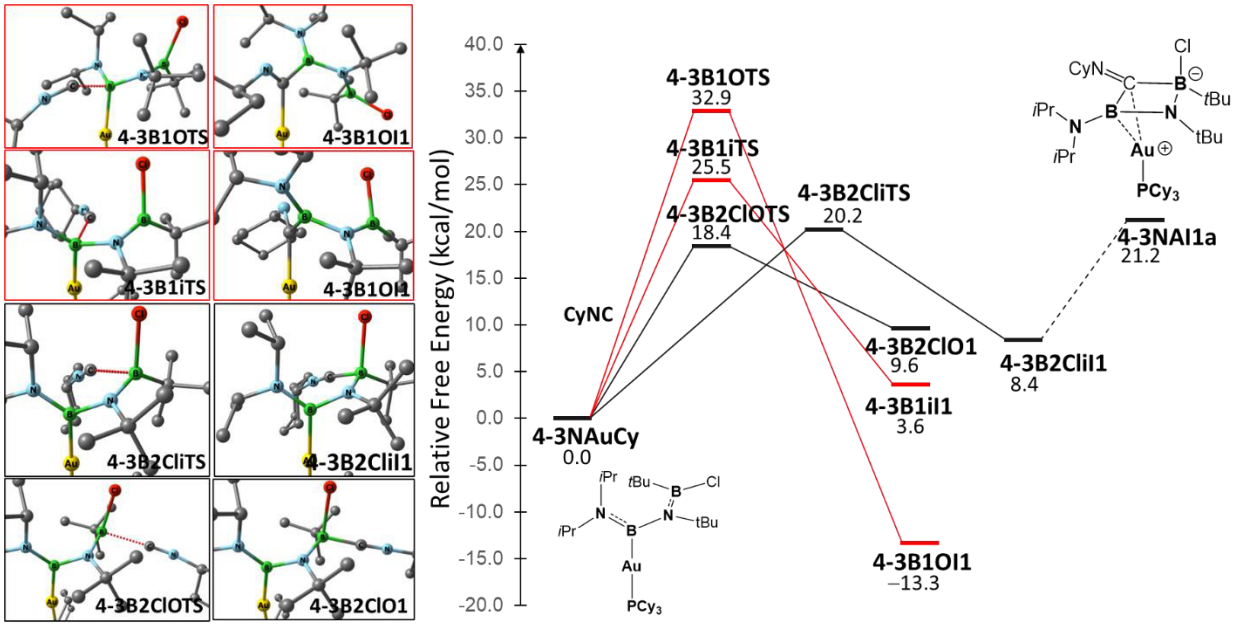


Figure 4-9. Calculated energetic profile of the addition of CyNC to **4-3NAuCy**.

Not only the outer addition of CyNC to boron bonded to chloride is plausible (**4-3B2ClOTS**) (**Figure 4-10**, blue line) but also the inner addition of CyNC, only when chloride atom is pointing in the direction of gold atom (**4-3NATS2**) (**Figure 4-10**, red line). The calculated total energy barrier of 18.4 kcal/mol competes with the direct addition pathway (**Figure 4-10**, blue line).

Overall, two different reaction paths favor the reaction of **4-3NAuCy** with CyNC. The first one, the outer addition of CyNC to boron bonded to chloride (**4-3B2ClOTS**, $\Delta G_{1B}^{\ddagger}$ = +18.4 kcal/mol) generates intermediate **4-3B2ClO2** (ΔG_{R1B} = +9.6 kcal/mol) which can lead to

conformer **4-3NAI2** (ΔG_{R1B} = −1.5 kcal/mol) just by rotating the B–N bond. For the second one, the (Cl)(*t*Bu)B=N(*t*Bu)(R) bond must rotate (**4-3NATS1**, $\Delta G_{1R}^{\ddagger}$ = +15.6 kcal/mol) producing **4-3NAI1** (ΔG_{R1R} = +2.3 kcal/mol). Then, addition of CyNC to the boron bonded to chloride occurs (**4-3NATS2**, $\Delta G_{1R}^{\ddagger}$ = +16.1 kcal/mol) leading to **4-3NAI2** (ΔG_{R2R} = +5.8 kcal/mol). Now that the reaction paths converge in intermediate **4-3NAI2**, gold atom attacks carbon of CyNC (**4-3NATS3**, $\Delta G_{1}^{\ddagger}$ = +3.4 kcal/mol) forming the four-membered ring **4-3NAI3** (ΔG_{R1} = −4.2 kcal/mol). Our proposal is that this intermediate **4-3NAI3** is more stable than **4-3NAI1a** (**Figure 4-9**) due to less steric repulsion between the lone pairs of electrons of chloride atom and the *t*Bu groups. After that, bond C–B1 breaks (**4-3NATS4**, $\Delta G_{2}^{\ddagger}$ = +5.6 kcal/mol) producing **4-3NAI4** (ΔG_{R2} = −8.6 kcal/mol). Finally, migration of carbon to the second borane proceeds trough transition state **4-3NATS5** (**Figure 4-11**) ($\Delta G_{3}^{\ddagger}$ = +16.4 kcal/mol) forming **4-5NACyI** (ΔG_{R3} = −17.9 kcal/mol). Cyclization of **4-3NAI4** is not favored because it has an energy barrier of 19.0 kcal/mol (**4-3NATS6**) which is 2.6 kcal/mol higher than the carbon migration **4-3NATS5**. In addition, this reaction is done at −30°C experimentally and the calculated total energy barrier is of 18.4 kcal/mol, which is quite high for the given temperature. Therefore, the reaction mechanism must be calculated at this temperature to further corroborate.

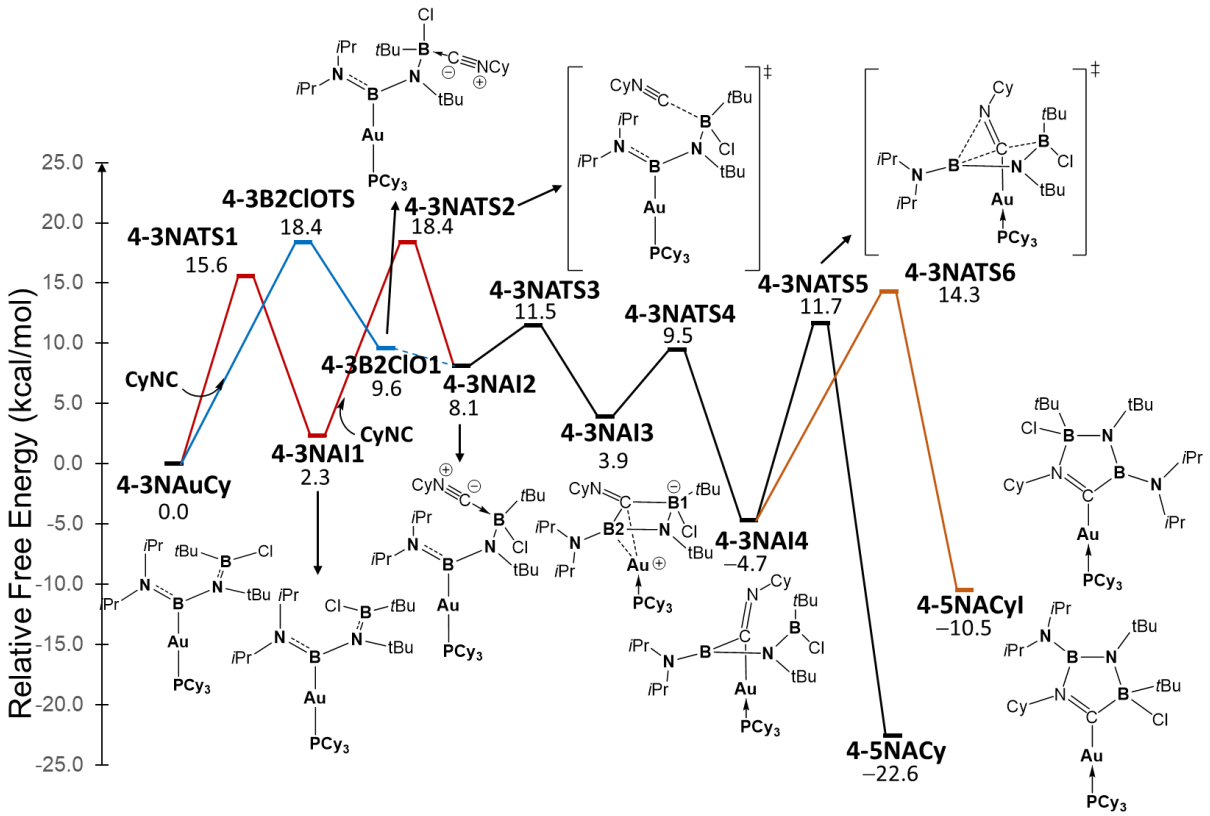


Figure 4-10. Proposed reaction mechanism of –NiPr2 gold(I) derivative (**4-3NAuCy**) with CyNC.

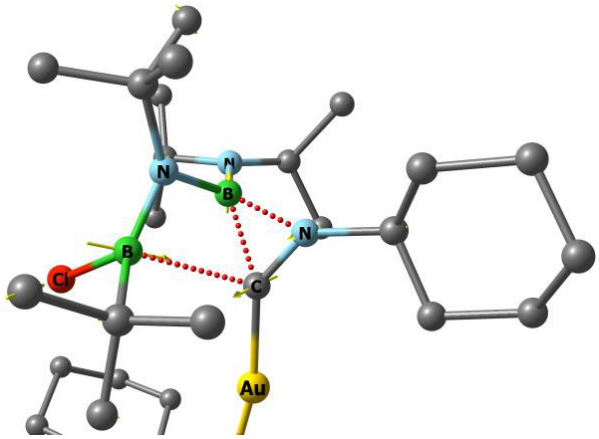


Figure 4-11. Optimized transition state **4-3NATS5**. Phosphine and hydrogens are not shown for clarity.

Indeed, the calculated reaction mechanism at –30°C (or 243 K) (**Figure 4-12**) lowers the total energetic barrier from 18.4 to 16.2 kcal/mol. Even the energies of the transition states **4-3B2ClOTS** and **4-3NATS2** lowers from 18.4 kcal/mol to 16.3 and 16.1 kcal/mol, respectively.

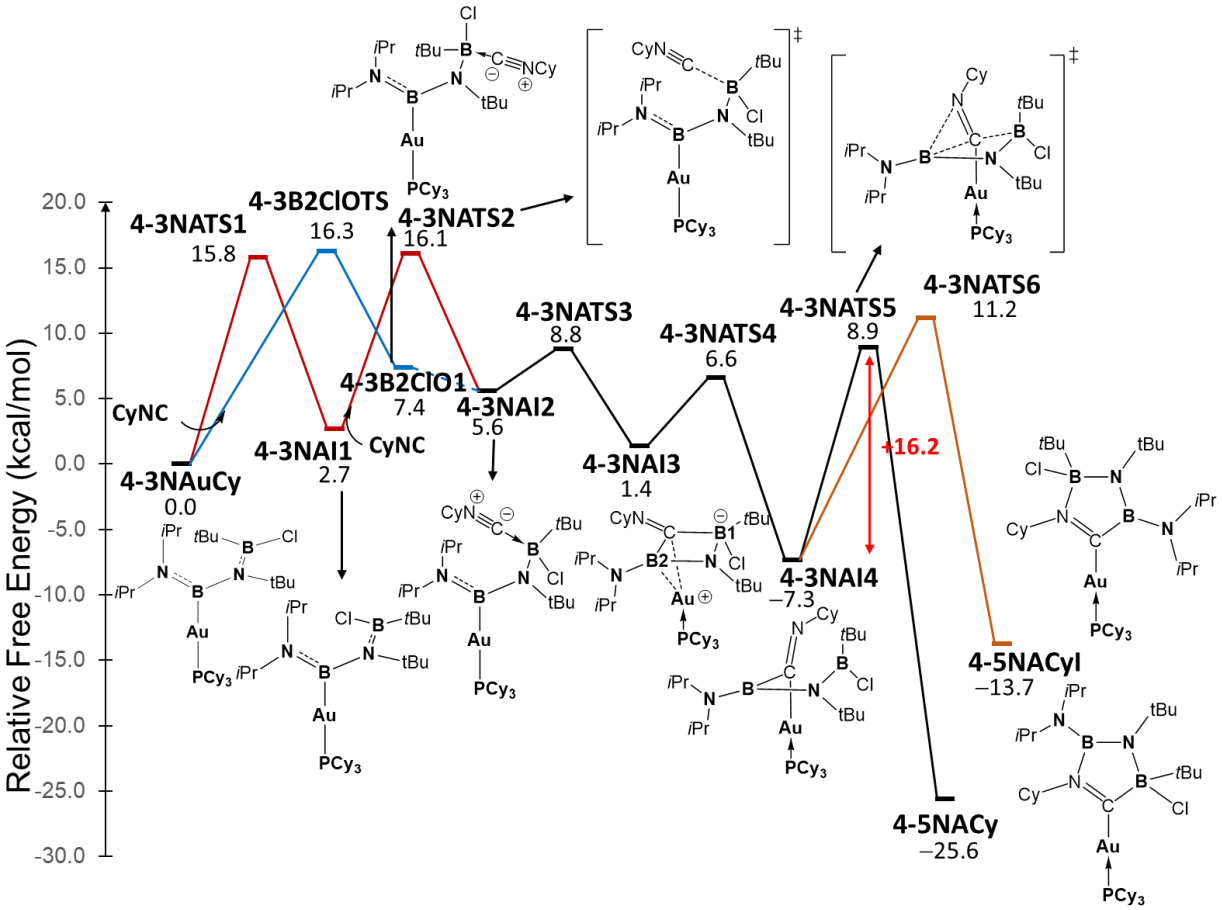


Figure 4-12. Proposed reaction mechanism of –NiPr2 gold(I) derivative (**4-3NAuCy**) with CyNC calculated at 243°C.

Moreover, if the previous reaction is heated up to room temperature for 4 days, the reaction proceeds slowly towards the migration of the *t*Bu group to the carbon carbene (**4-5NACyM**). The calculated transition state consists in a 3c–2e bond between carbon of *t*Bu, boron and carbon of carbene (**Figure 4-13**) and the calculated reaction step has a barrier energy of 24.2 kcal/mol and is exergonic (ΔG°_{R} = −11.3 kcal/mol) which agrees with the experimental conditions.

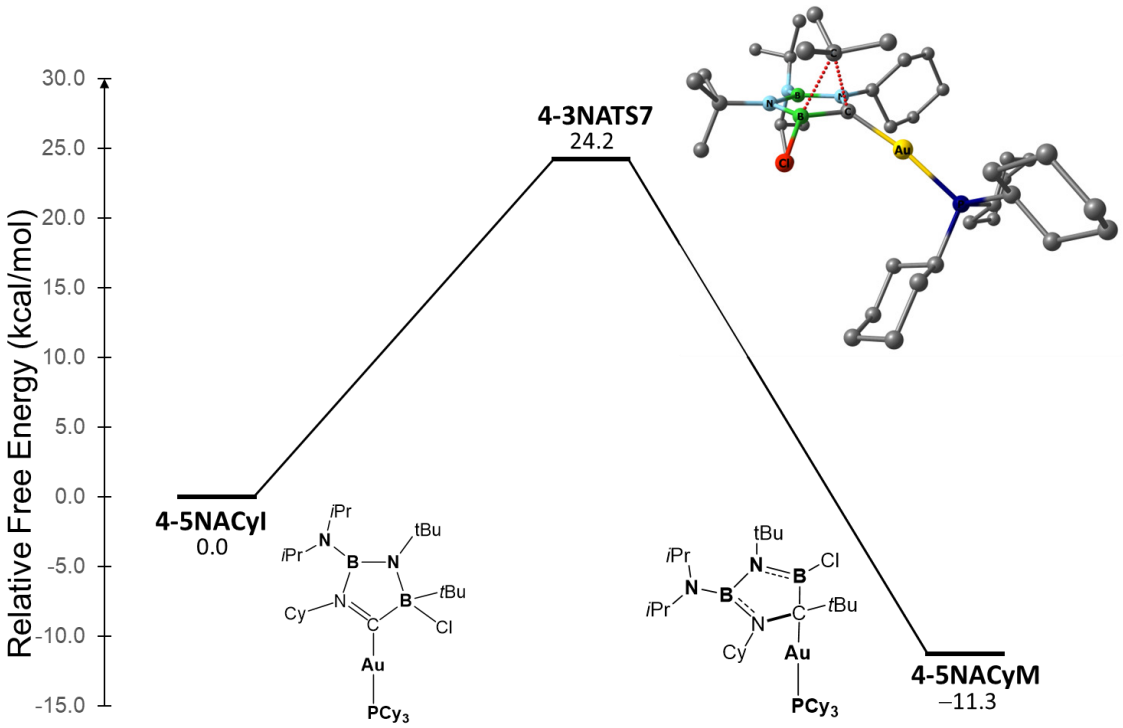


Figure 4-13. Energy profile of the *t*Bu migration in complex **4-5NACyI**.

The cationic reaction mechanism was also considered for the reaction of **4-3NAuCy** with CyNC. In **Figure 4-14** only the relevant reaction steps are shown. First, because the solvation energies for the ion chloride in benzene are not available in the literature, an approximation was used: the ion chloride solvation energies in 1,2-dimethylether (DME) and in ethanol were used instead.[74] For the ethanol case, the dissociation of chloride from **4-3NAI2** to **4-3NP1** is exergonic (ΔG_{EtOH} = −1.3 kcal/mol) but introducing the less polar solvent 1,2-dimethylether (DME) the dissociation becomes endergonic (ΔG_{DME} = +5.6 kcal/mol). Therefore, a polar solvent may induce the reaction to take the dissociative reaction pathway. After the chloride dissociation, gold atom attacks the carbocation (**4-3NTS1**, $\Delta G_1^{\ddagger}$ = +4.5 kcal/mol) leading to the four-membered ring **4-3NP2** (ΔG_{R1} = −1.3 kcal/mol). Then, the bond C–B2 breaks (**4-3NTS2**, $\Delta G_2^{\ddagger}$ = +13.7 kcal/mol) and leads to a boracation **4-3NP2** (ΔG_{R2} = +11.3 kcal/mol) which is highly stabilized by the two adjacent nitrogens. Finally, cyclization occurs (via transition state **4-3NTS3**, $\Delta G_3^{\ddagger}$ = +5.6 kcal/mol) and leads to the cationic BNC gold(I) complex **4-3N4** (ΔG_{R3} = −32.7 kcal/mol). Overall, for all the compounds in the cationic mechanism, except chloride ion, the solvation energies are calculated for benzene. We expect that a polar solvent may diminish the

total energy barrier of 16.9 kcal/mol and favors the chloride dissociation of **4-3NAl2**, inducing the cationic reaction mechanism.

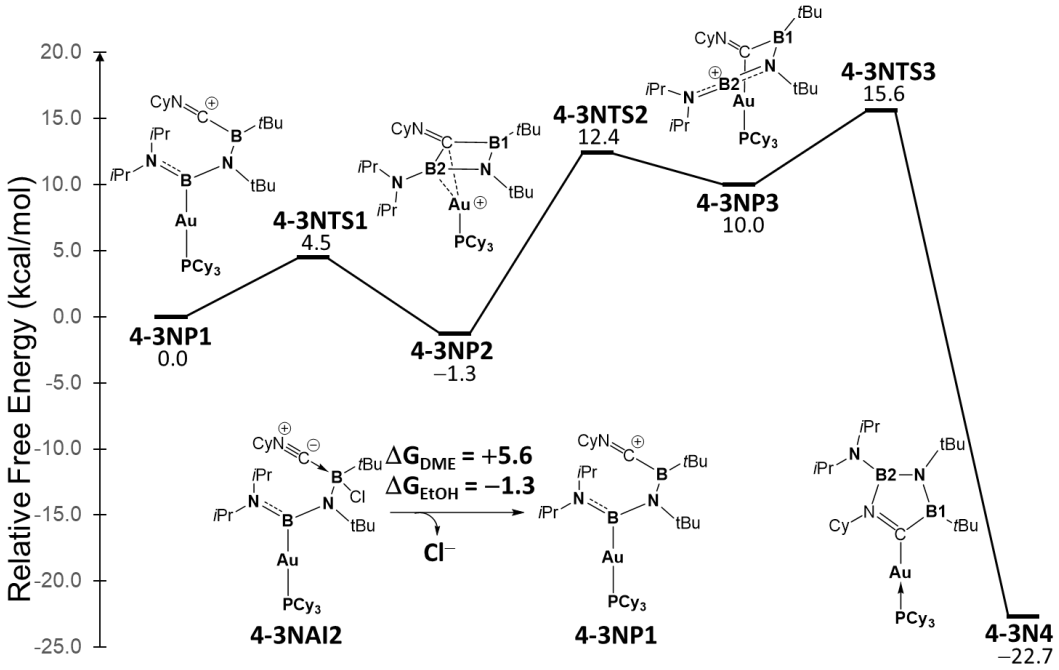


Figure 4-14. Cationic pathway of the reaction of **4-3NAuCy** with CyNC.

4.3. BNC carbene gold(I) reactions

BNC gold(I) complexes such as **4-5tCl** can be further react with AgOTf to form **4-5tOTf** or with lithium to reduce it to **4-5tLi** (**Figure 4-15**). Each of these products have an interesting chemical question. For **4-5tOTf**: why the coordination of triflate remains in solid state and even in solution? For **4-5tLi**: where the reduction occurs, at the gold atom or at the heterocyclic ring? These are the questions that we are going to answer in this section.

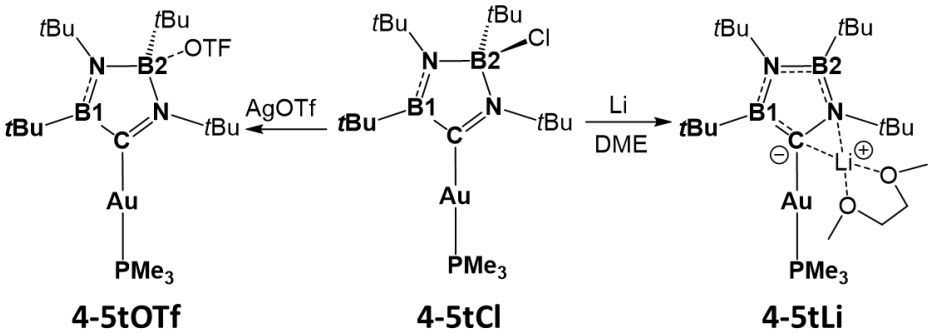


Figure 4-15. BNC gold(I) complex **4-5tCl** reduction and reaction with AgOTf.

4.3.1. Analysis of 4-5tOTf

Two ^{11}B NMR signals were expected for **4-5tOTf**, nevertheless the signals were unobserved. Sometimes this is due to a fluxional process involved in the complex. Therefore, we hypothesized that in solution **4-5tOTf** the triflate may dissociate or migrate to the other boron (B1). Indeed, according to our calculations, complex **4-5tOTF** has a plausible fluxional behavior where the triflate is migrating from boron (B1) to boron (B2) (**Figure 4-16**). To begin with, triflate of **4-5tOTf** dissociates from boron (B1) via transition state **4-5OtfTS1** ($\Delta G_1^{\ddagger}$ = +16.1 kcal/mol) and it generates ion pair **4-5tOTfI1** (ΔG_{R1} = +9.1 kcal/mol) (**Figure 4-17**). The triflate again coordinates the second boron (B1) (**4-5OtfTS2**, $\Delta G_2^{\ddagger}$ = +5.4 kcal/mol) and leads to isomer **4-5tOTfIs** (ΔG_{R1} = −7.6 kcal/mol). The overall reaction is endergonic with a reaction energy of +1.5 kcal/mol and has a barrier energy of 16.1 kcal/mol. This indicates a favored fluxional process of the migration of the triflate from boron (B2) to boron (B1). Moreover, the fully dissociation of **4-5tOTfI1** into the anion triflate and the cationic BNC gold(I) complex (**4-5tP**) is unfavored due to the high dissociation energy of 22.6 kcal/mol. Therefore, this fluxional process must involve ion pair **4-5tOTfI1**. From this calculation, it is concluded that the cationic ring of complex **4-5tP** is highly unstable and that triflate tends to bond with any of the borons.

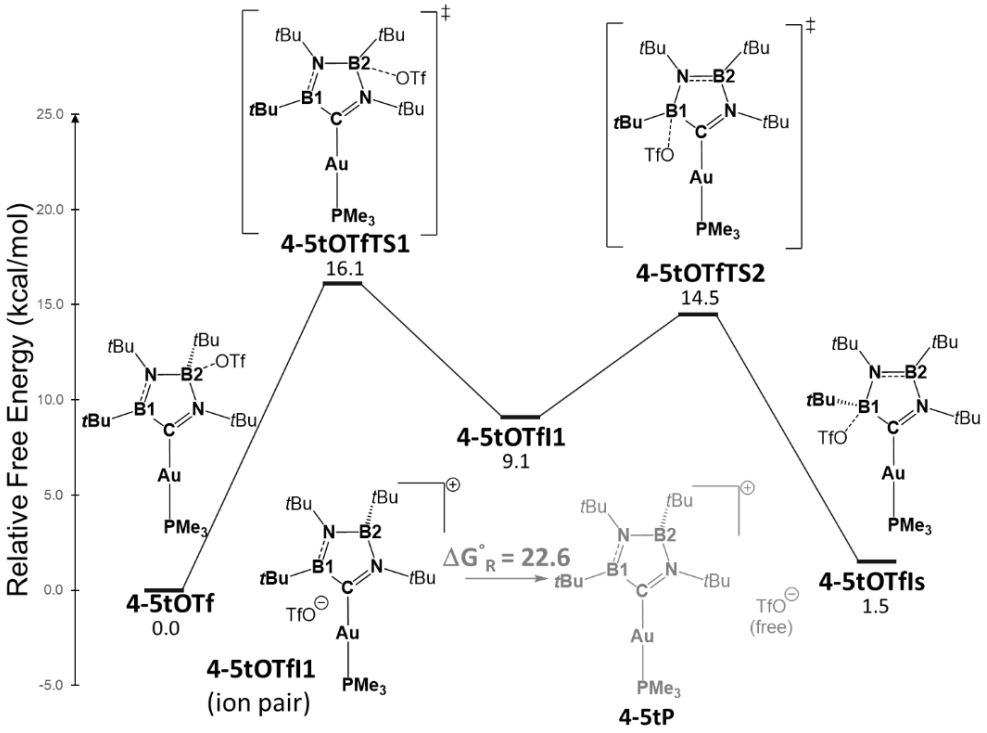


Figure 4-16. Plausible fluxional process for the triflate migration from boron (B2) to boron (B1).

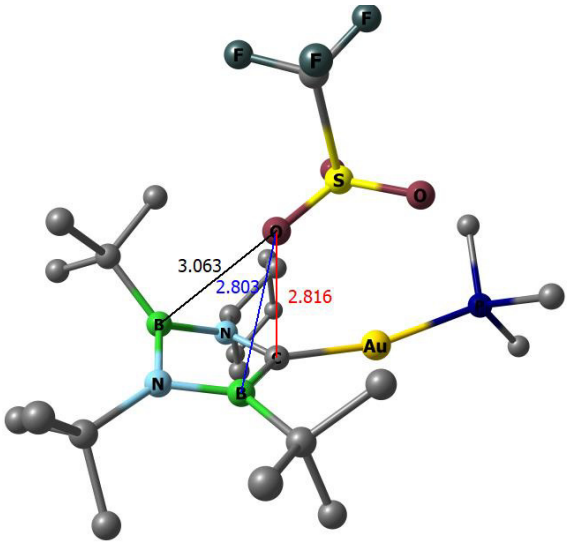


Figure 4-17. Optimized geometry of ion pair **4-5tOTfI1**. Relevant distances are given in armstrong (Å).

To further investigate the instability of cationic complex **4-5tP**, a Nucleus Independent Chemical Shift (NICS) was performed. This method measures the induced electromagnetic field in a point that is placed perpendicular to the ring plane of the system (usually a ghost atom is used) and can be used to determine aromatic, antiaromatic and non-aromatic systems if the NICS profile contains only negative, positive and values close to cero respectively. Overall, the NICS profile of **4-5tP** (**Figure 4-18**) has positive and negative NICS values, with a NICS(0) = +2.64 and a NICS(1) = –1.06, indicating a non-aromatic ring.

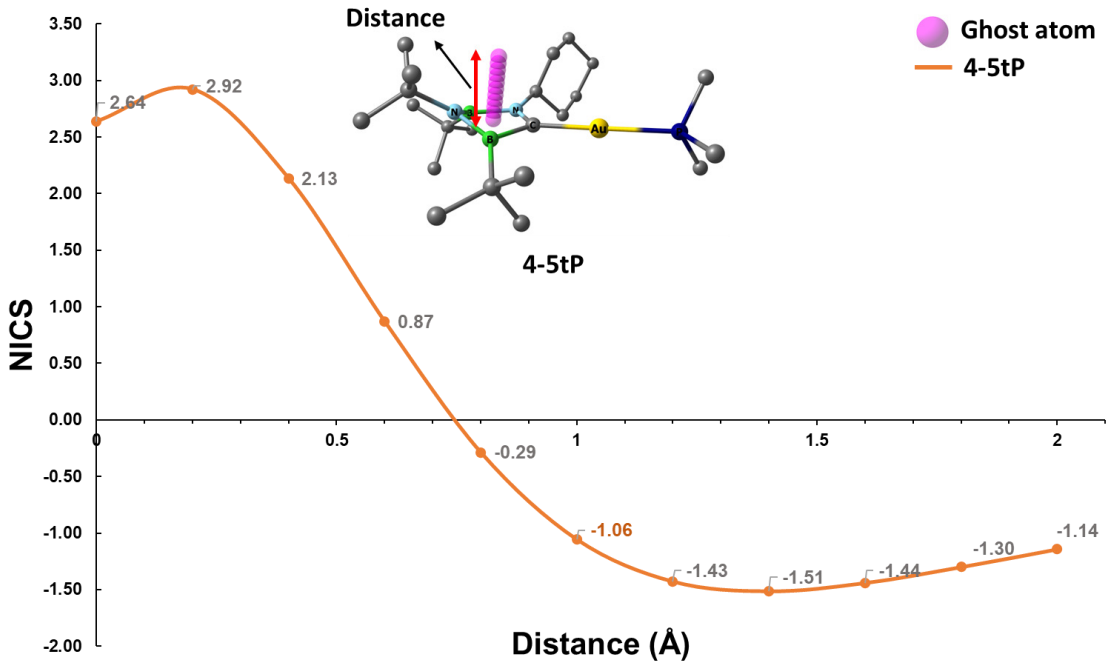


Figure 4-18. NICS profile of **4-5tP**.

Moreover, the anisotropy of the induced current density (ACID) methodology was calculated for **4-5tP**. This method also allows to determine aromatic, antiaromatic and non-aromatic systems and can be assigned depending on the flow of the current density vectors plotted into the ACID surface: clockwise and counterclockwise indicate that the ring is aromatic or antiaromatic respectively. If the flow of the current density vectors is not uniform towards the clockwise or counterclockwise direction, then the system is non-aromatic. This is the case for complex **4-5tP**, the current density vectors do not flow uniformly (see **Figure 4-19**, red arrows). Therefore, the heterocyclic ring of **4-5tP** is non-aromatic and agrees with the NICS calculations.

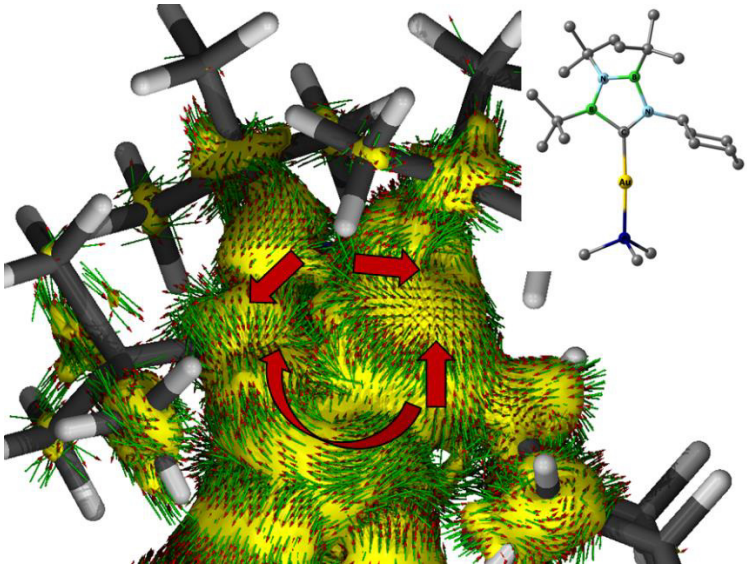


Figure 4-19. ACID isosurfaces of **4-5tP**. Current density vectors are plotted onto the ACID surfaces.

4.3.2. Analysis of 4-5tLi

The product (**4-5tLi**) of the reduction reaction of **4-5tCl** with lithium has not a trivial electronic structure because Bertrand reported a similar reduction and in their results they show that the gold center is the one reduced,[51] however, one year after their publication, F. Weinhold reported that the one reduced is the carbene ring and not the gold center[52] (for more details see **CHAPTER 1**, 1.2.4, **gold carbene reduction**). Therefore, the calculations that we applied here are similar to those performed by F. Weinhold.

To analyze the bonding mechanism of **4-5tLi** the natural bond orbitals (NBO) and intrinsic bond orbitals (IBO) methods were used (see **CHAPTER 2** for theoretical details). Both methods give the same results: the heterocyclic ring is the one reduced.

NBO analysis shows that heterocyclic ring of **4-5tLi** contains 6 π-electrons (**Figure 4-20**). A π-bond is calculated between boron (B1) and carbon carbene (NBO **A**). Therefore, the electron lone pair of nitrogen no longer stabilizes the empty *p*-orbital of carbon carbene (NBO

B). The last 2π electrons are localized in the double bond between the upper nitrogen and boron (B2) (NBO **C**). Moreover, the electrons in the π-bond between boron (B1) and carbon carbene (NBO **A**) are more localized in carbon (76.01 %) than in boron (23.99 %), indicating that the reduction fills the empty *p*-orbital of carbon carbene (**Scheme 4-2**) and this pair of electrons delocalize towards the adjacent boron resulting in NBO **A**.

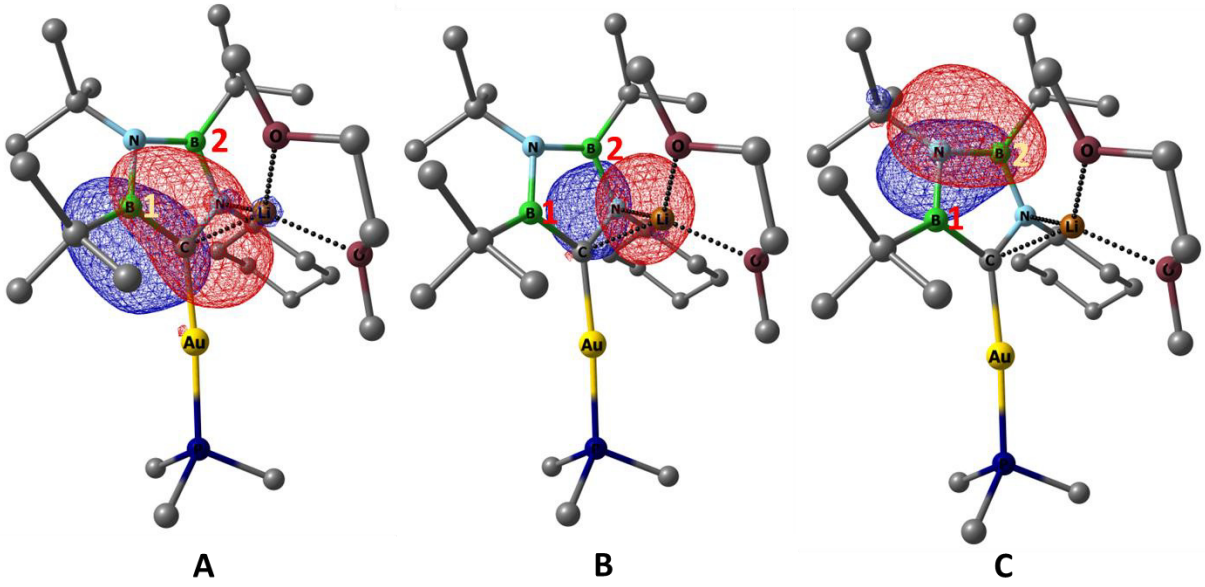
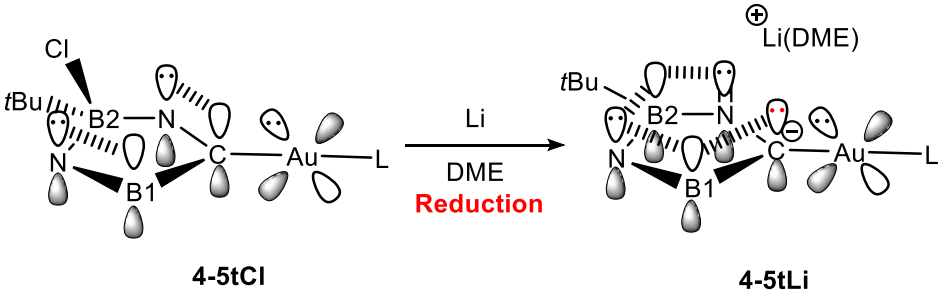


Figure 4-20. Relevant NBOs of **4-5tLi** (isosurface = 0.03).



Scheme 4-2. Representation of valence orbitals of relevant atoms in **4-5tCl** and **4-5tLi**.

An IBO analysis gives the same chemical bonding pattern then NBO. Nevertheless, NBO calculates the bond pattern based on the best Lewis structure gotten through their algorithm. IBO calculations can also be assimilated with Lewis structure but the resulting IBOs are not restricted to the best Lewis structure. Therefore, bond delocalizations are taken more into account. For example, in **Figure 4-21** IBO **B** shows a delocalization of the lone pair of nitrogen towards the adjacent boron, meanwhile NBO **B** (**Figure 4-20**) analog only shows a lone pair of electrons and in IBO **C** the lone pair of nitrogen is delocalized towards both borons and NBO **C** is only delocalized towards one boron.

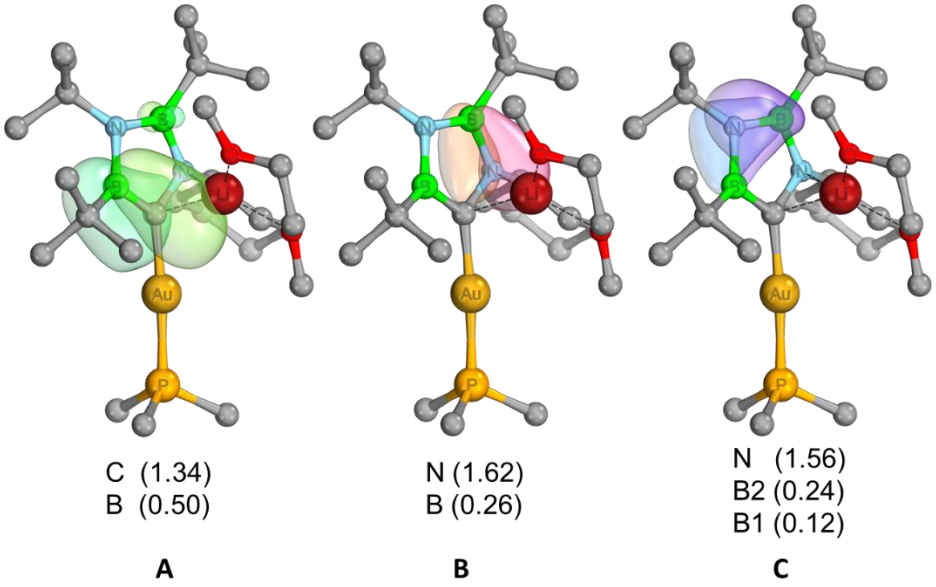


Figure 4-21. Relevant IBOs of **4-5tLi**.

In general, IBO and NBO calculations for complex **4-5tLi** show that the reduction fills the empty *p*-orbital of carbon. Considering this electron lone pair of carbon and the two lone pairs of the two nitrogens give a total of 6 π-electrons (**Scheme 4-2**), this indicates that the ring is aromatic.

A NICS profile calculation of **4-5tLi** corroborates that the heterocyclic ring is indeed aromatic with values of NICS(0) and NICS(1) of –6.22 and –3.51 (**Figure 4-22**, orange line). Even if the lithium cation and the dimethoxyethane are removed, the heterocyclic ring maintains its aromaticity. However, the NICS(0) value increases to –4.47 and NICS(1) of –3.51 slightly diminishes (**Figure 4-22**, blue line), meaning that the heterocyclic ring is more aromatic when lithium is coordinated (**4-5tLi**). Therefore, lithium cation helps to delocalize electron density in the heterocyclic ring of **4-5tLi**.

Moreover, an ACID calculation also corroborates the aromaticity in ring **4-5tN**. In **Figure 4-23** the current density vectors plotted onto the ACID surface of the heterocyclic ring of **4-5tN** show a clockwise rotation, characteristic of an aromatic ring.

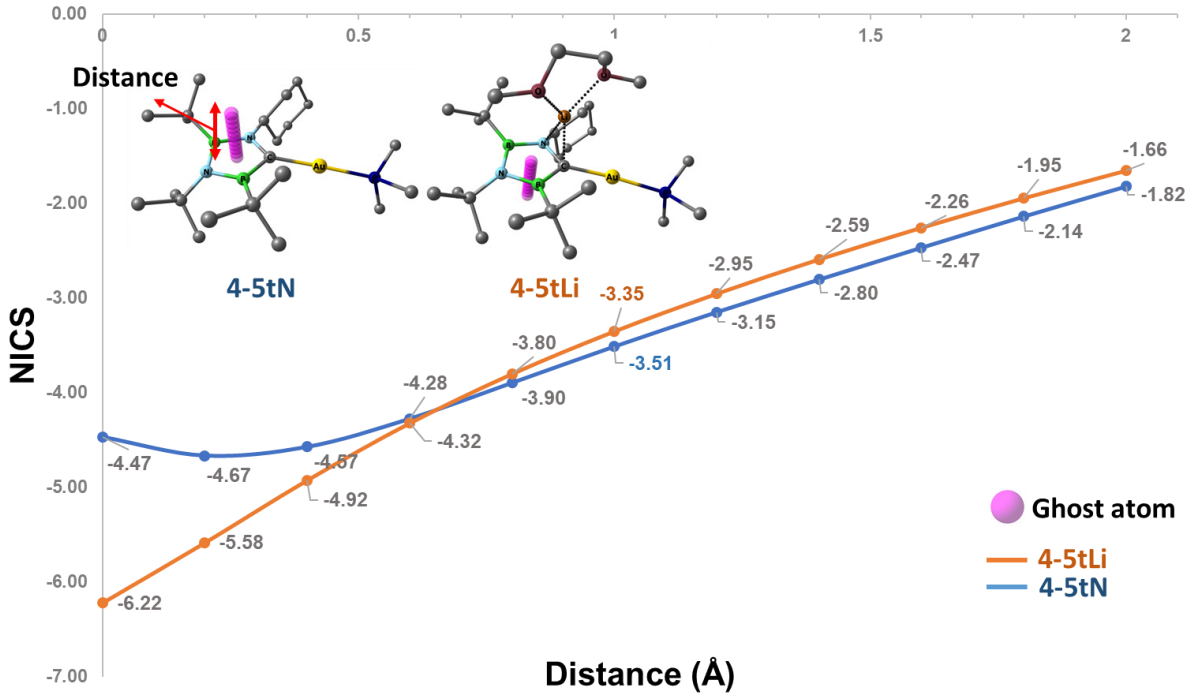


Figure 4-22. NICS profile of **4-5tN**.

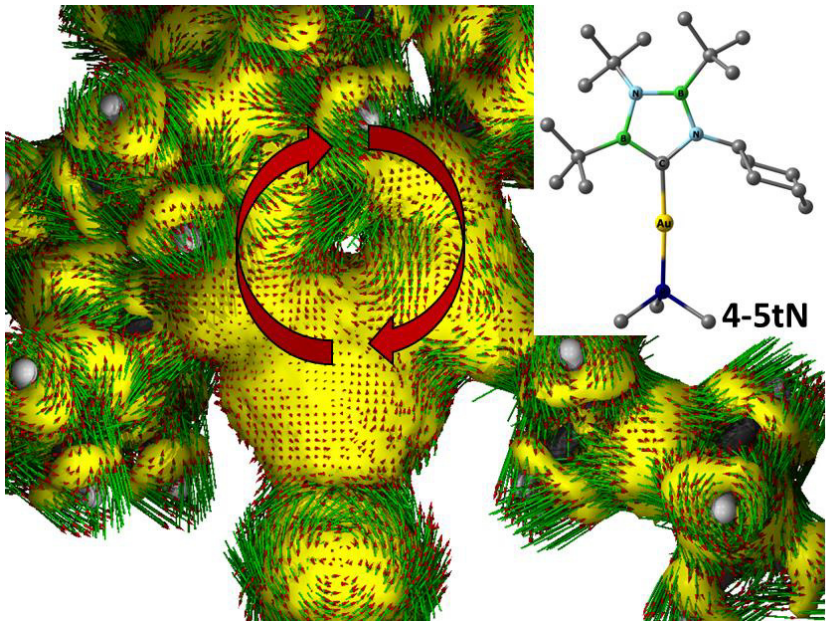


Figure 4-23. ACID isosurfaces of **4-5tN**. Current density vectors are plotted onto the ACID surfaces.

4.3.3. Walsh diagram 4-5tP and 4-5tN

The bonding mechanism not only can be explained in terms of IBO calculations but also with Molecular Orbitals (MOs). In specific, the Walsh diagram of cationic and anionic BNC gold(I) complexes, **4-5tP** and **4-5tN**, allows to understand which MOs of the BNC carbene and gold fragments interacts to form the MOs of the complex.

According to the Walsh diagram of the BNC carbene gold complex **4-5tP** (**Figure 4-24**), HOMO is formed from LUMO of the gold fragment $[Au\text{-}PMe_3]^+$, which can be associated with a gold *sp* hybrid orbital, and the HOMO of BNC carbene fragment, that corresponds to the lone pair of carbene. LUMO of the complex is only produced by LUMO of BNC carbene with the feature that this complex MO is mostly located at the BNC carbene moiety. LUMO+1 of the complex corresponds to two degenerate gold *6p*-orbitals. The shape of these orbitals are almost equal to the ones calculated for the gold fragment (LUMO+1 of $[Au\text{-}PMe_3]^+$), indicating that the mix of these gold orbitals with the BNC carbene orbitals are not favored. Moreover, the two-electron reduction of **4-5tP** will fill the LUMO of this complex, and because this LUMO is located at the BNC carbene moiety, the reduction would occur at this site.

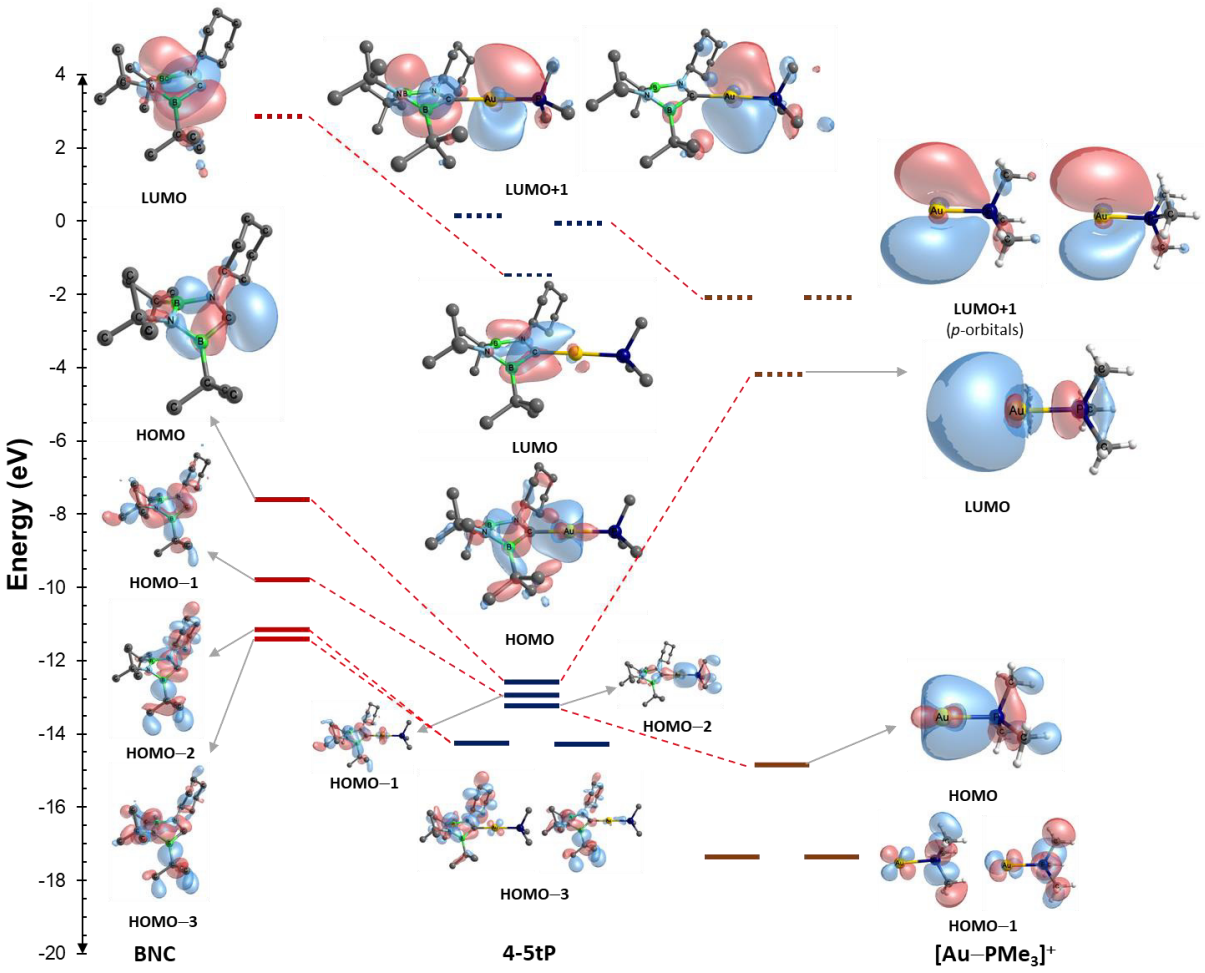


Figure 4-24. Walsh diagram of **4-5tP**.

The Walsh diagram of anionic BNC carbene gold complex **4-5tN** explains whether the electron reduction occurs at the BNC carbene moiety or at the gold atom. Herein, the HOMO of **4-5tN** is formed by the HOMO of the dianionic BNC carbene fragment $(BNC)^{-2}$. Because the complex HOMO is mainly located at the carbene moiety, it indicates that the reduction occurs at this site. The formation of the LUMOs and HOMO-1 can be explained in a similar way as it was previously done for **4-5tP** (**Figure 4-24**). Even though, the complex frontier MO does not give qualitative evidence of an interaction between the BNC carbene moiety and the gold atom, other type of methods, such as the analysis of NBO donor-acceptor interactions, can quantify the interaction between these sites.

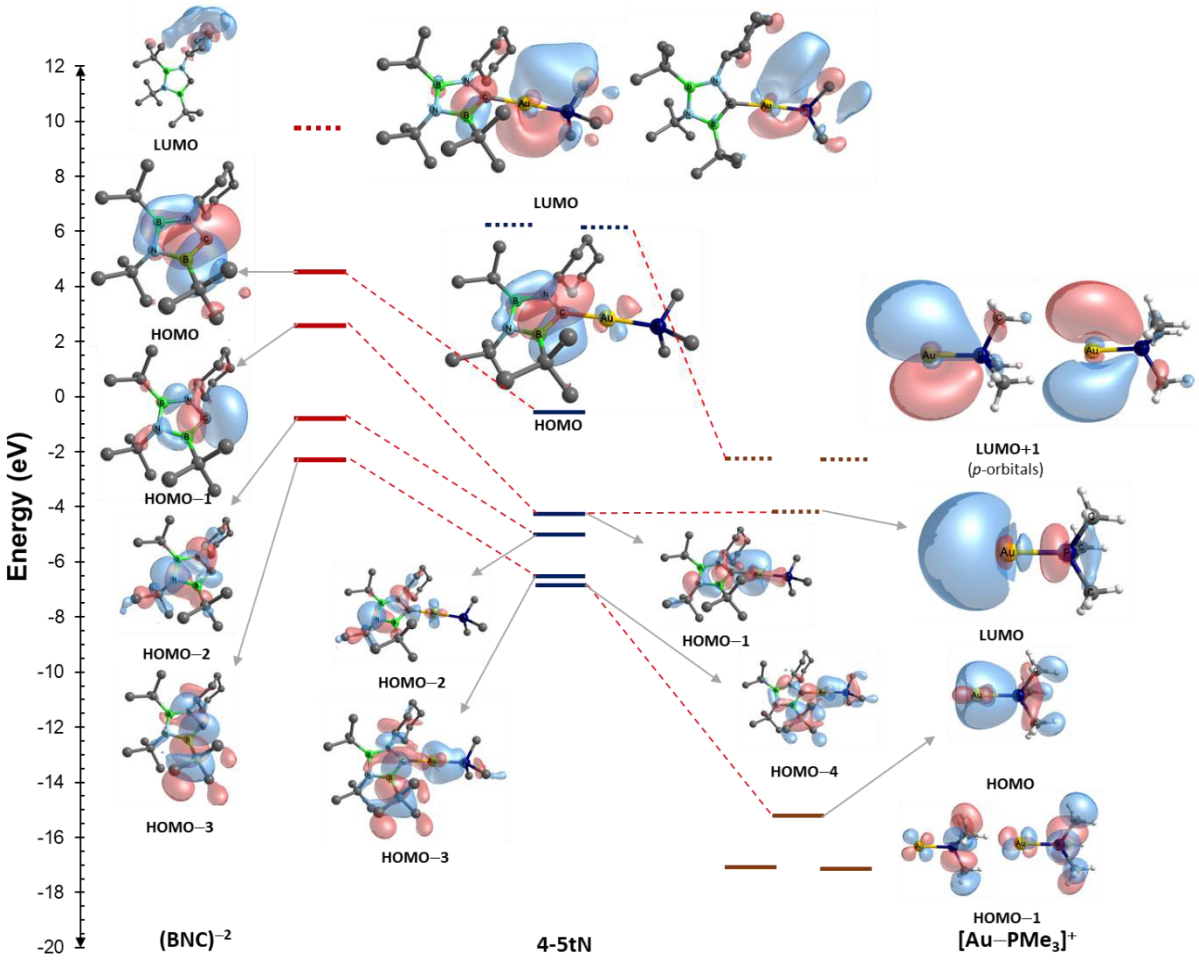


Figure 4-25. Walsh diagram of **4-5tN**.

4.4. Properties of BNC gold(I) complexes

4.4.1. Comparison of free BNC carbene among NHC and CAAC carbenes

Before the comparison of BNC (B,N-heterocyclic Carbenes) carbene gold(I) complexes among other gold(I) carbenes is presented, the differences among free BNC, NHC and CAAC carbenes are discussed in this section.

As mentioned in the introduction, the σ–donating and π–accepting properties of carbenes can be compared, generally, in terms of their HOMO and LUMO energies. HOMO must correspond to the lone pair of electrons of carbon carbene (E_σ) and LUMO to the π*(C–N) antibonding orbital ($E_\pi*$), see **Figure 4-26**. Higher E_σ energies indicate that the carbene is better σ–donating and lower $E_\pi*$ shows that it is better π–accepting (see **CHAPTER 1**, **1.2.3**).

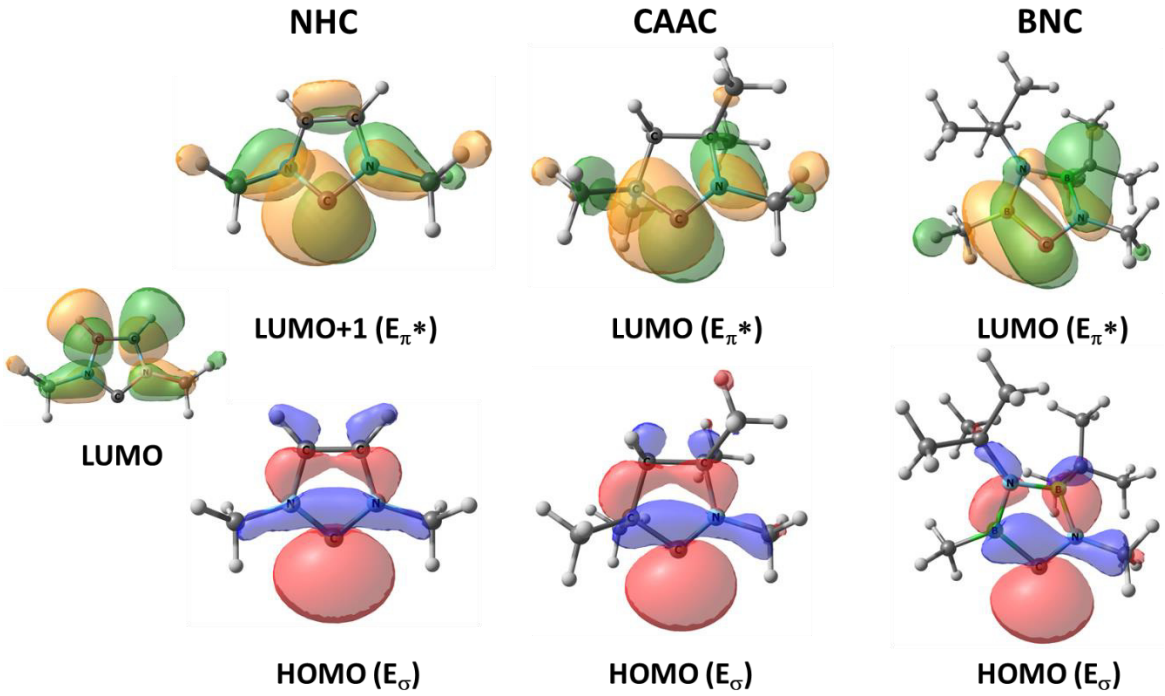


Figure 4-26. Relevant Molecular Orbitals of **NHC**, **CAAC** and **BNC** that correspond to E_σ and $E_\pi*$.

The calculated energies of relevant molecular orbitals of **NHC**, **CAAC** and **BNC** (**Figure 4-27**) reveals that the σ–donating properties of these carbenes follow the trend of: **NHC** ($E_\sigma = -7.86$ eV) < **CAAC** ($E_\sigma = -7.26$ eV) < **BNC** ($E_\sigma = -6.79$ eV), and the π–accepting properties follow the order of: **NHC** ($E_\pi* = 3.42$ eV) < **CAAC** ($E_\pi* = 2.27$ eV) < **BNC** ($E_\pi* = 0.35$ eV). Overall, this indicates that BNC carbene is the most σ–donor and π–acceptor.

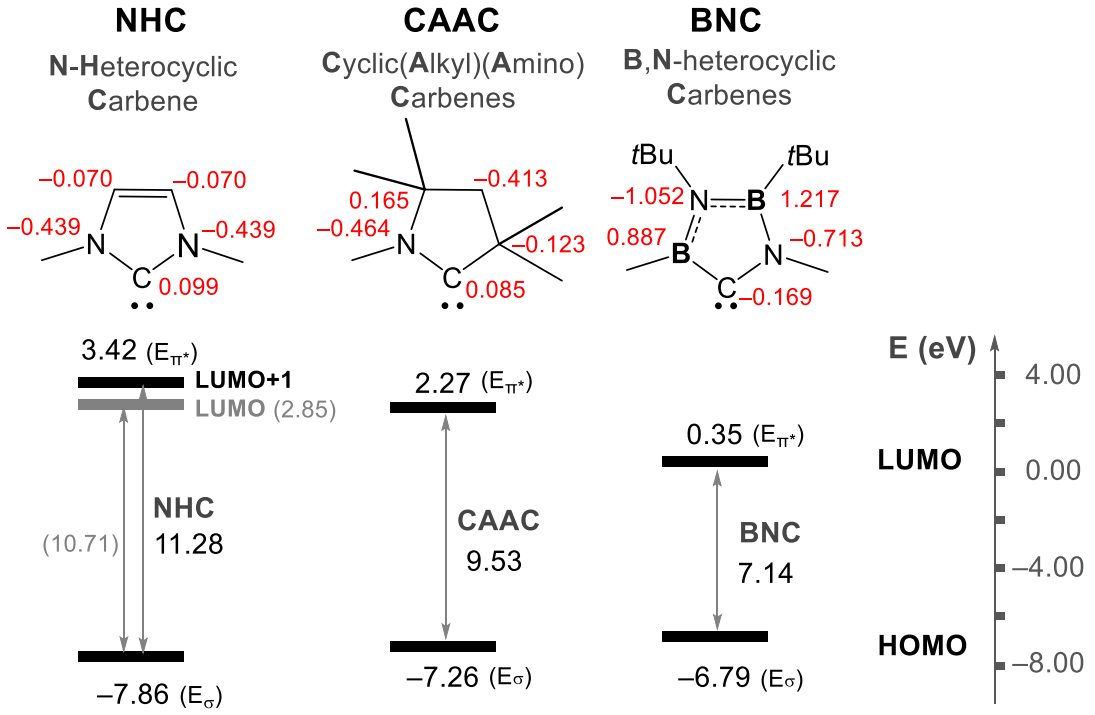


Figure 4-27. E_σ and $E_{\pi*}$ energies (eV) of general NHC, CAAC and BNC free carbenes. NBO charges are labeled in red color.

The NBO charges gives a hint on why BNC is the most σ–donating among NHC and CAAC carbenes (**Figure 4-27**, red numbers). Among these carbenes, BNC has the most negative charge in carbon carbene of –0.169 e^-, and this is expected as the carbon carbene is bonded to a boron, which is more electropositive than carbon or nitrogen. This boron can give electron density to the carbene, and thus increases the σ–donating properties.

To evaluate why BNC is a highly π–accepting carbene, NBO calculations were performed in specific Lewis structures that do not form a π(C–N) bond (**Figure 4-28**) so the electron population of the *p*-orbital of carbon carbene can be evaluated.

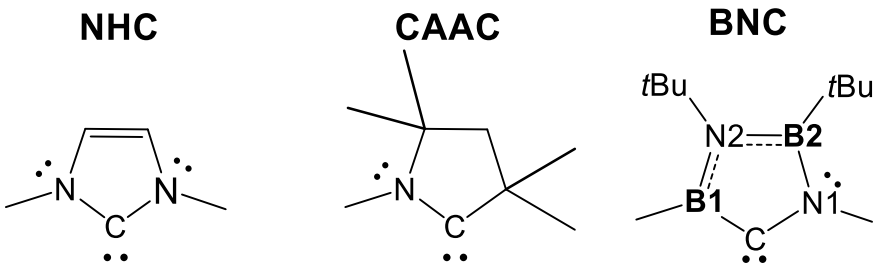


Figure 4-28. Selected Lewis structures of NHC, CAAC and BNC to perform an NBO calculation to evaluate the π–accepting properties.

The calculated electron population in carbene of **NHC**, **CAAC** and **BNC** (**Table 4-1**) also follows the same trend as the energies of the molecular orbitals in how the π–accepting properties increases. The more the electron population diminishes, the more the π–accepting properties increases. **NHC** has the most electron population in the *p*-orbital of carbene (0.6433 e^-) and this is anticipated because the lone pair of each of the two adjacent nitrogens delocalizes into this *p*-orbital. The electron population of the carbon carbene *p*-orbital diminishes in **CAAC** (0.4503 e^-) as it only contains one adjacent nitrogen. **BNC** has the lowest electron population in the *p*-orbital of carbon carbene (0.4085). According to NBO, this is mainly due to the ability of the lone pair of electrons of nitrogen (N1) to delocalize also to the empty *p*-orbital of boron (B2) (*p*(N1)→*p*(B2)). The calculated interaction energy (E(2)) of *p*(N1)→*p*(B2) is 35.07 kcal/mol (**Figure 4-29**, **A**) which is low compared to the interaction energy (E(2)) of *p*(N1)→*p*(C) which is 178.57 kcal/mol (**Figure 4-29**, **B**). The ratio of these energies indicates that the lone pair of nitrogen is five times more delocalized to the empty *p*-orbital of carbon carbene than to the empty *p*-orbital of boron (B2). Although the delocalization to boron (B2) is low, it improves the π–accepting properties of **BNC**.

Table 4-1. Amount of electrons delocalized of the lone pair of electrons of nitrogen/s to the *p*-orbital of carbon/boron of **NHC**, **CAAC** and **BNC**.

	Carbon carbene *p*-orbital
NHC	0.6433
CAAC	0.4503
BNC	0.4085

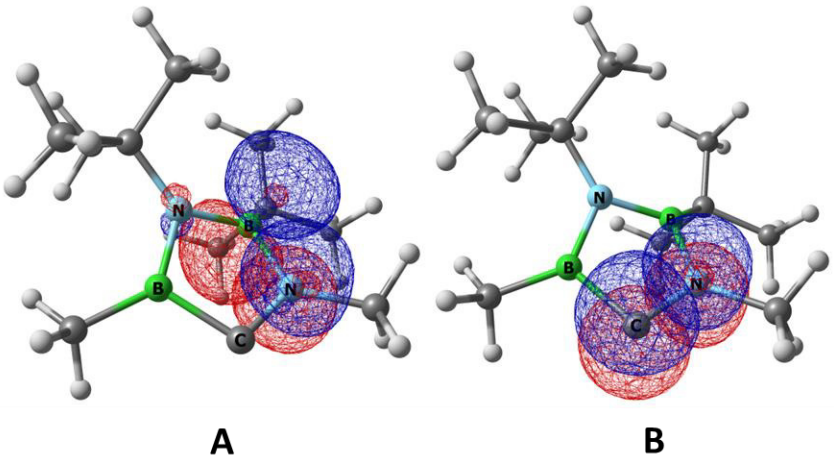


Figure 4-29. Donor-acceptor interaction of NBOs (A) p(N1)→p(B2) and (B) p(N1)→p(C).

4.4.2. Comparison of the π–accepting properties of a cationic BNC gold(I) complex among other complexes

The NBO second perturbation theory analysis allows to estimate the energy of the interaction (E(2)) between a donor orbital and an acceptor empty orbital. Therefore, it can be measured the interaction between a gold *5d*-orbital and the empty *p*-orbital of carbon carbene ($E_{Au\rightarrow C}$) (*d*(Au)→ *p*(C)) (**Figure 4-30**, **A**). The majority of the carbenes in **Table 4-2** contains an adjacent heteroatom to carbene, like a nitrogen. NBO calculates a bond between these atoms, hence, the interaction between NBOs *d*(Au)→π*(N-C) is used to measure $E_{Au\rightarrow C}$ (**Figure 4-30**, **B**). The higher this energy, the higher π–acceptor the carbene is.

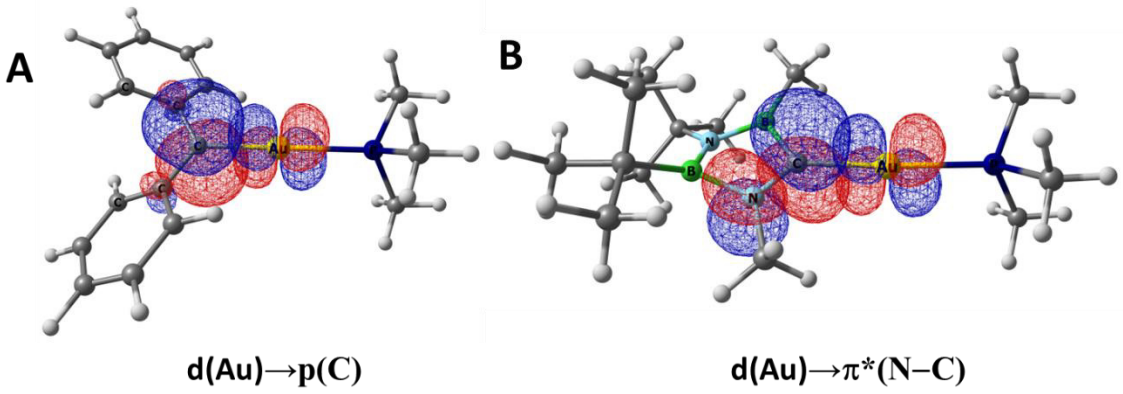
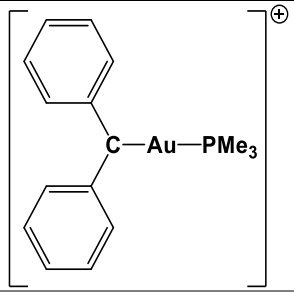
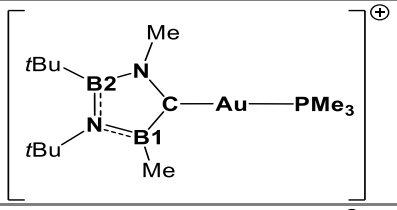
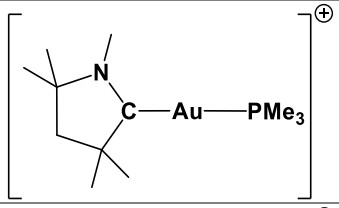
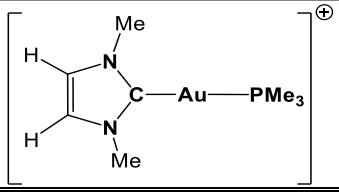


Figure 4-30. NBO donor-acceptor plots of a gold *d*-orbital and an orbital of carbon carbene of complexes (A) **$Ph_2CAuPMe_3$** and (B) **$BNCAuPMe_3$**.

Three different carbenes are used to compare the π–accepting properties of BNC gold(I) complex **$BNCAuPMe_3$** (**Table 4-2**), a CAAC, NHC and diphenylcarbene gold(I) complexes, **$CAACAuPMe_3$**, **$NHCAuPMe_3$** and **$Ph_2CAuPMe_3$** respectively. In **Table 4-2** all of these carbenes gold(I) complexes are ordered from the most π–acceptor to the lowest one according to their $E_{Au\rightarrow C}$ energies. Complex **$Ph_2CAuPMe_3$** is the most π–acceptor with an $E_{Au\rightarrow C}$ of 24.9 kcal/mol, and this is because it does not contain and adjacent heteroatom to the carbene that effectively stabilizes the empty *p*-orbital. Instead, the π electrons of benzene stabilize it (**Figure 4-31**). The value of this interaction is 82.3 kcal/mol for each benzene ring which is higher than $E_{Au\rightarrow C}$. The ratio of these interactions indicates that the benzene rings stabilize 6.6 times more than gold atom the empty *p*-orbital of carbon carbene. Complex **$BNCAuPMe_3$** is the most π–acceptor ($E_{Au\rightarrow C}$ = 15.6 kcal/mol) from the heterocyclic carbenes complexes **$CAACAuPMe_3$** ($E_{Au\rightarrow C}$ = 13.4 kcal/mol) and **$NHCAuPMe_3$** ($E_{Au\rightarrow C}$ = 12.7 kcal/mol), in agreement with previous calculations for the free carbenes.

Table 4-2. Donor-acceptor interaction energies (kcal/mol) of d(Au)→π*(N–C) ($E_{Au→C}$).

	Structure	$E_{Au→C}$ (kcal/mol)
$Ph_2CAuPMe_3$		24.9[1]
$BNCAuPMe_3$		15.6
$CAACAuPMe_3$		13.4
$NHCAuPMe_3$		12.7

[1]Donor-acceptor interaction energies calculated between d(Au)→p(C) ($E_{Au→C}$)

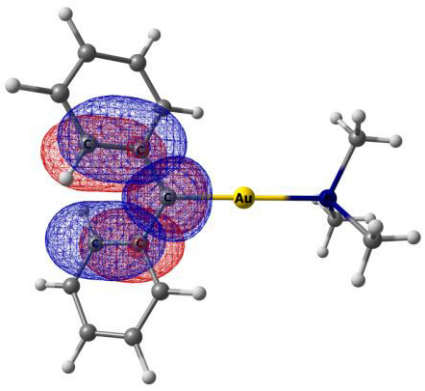


Figure 4-31. NBO donor-acceptor plot of NBOs π(C–C)→p($C_{carbene}$) from both benzene rings.

4.4.3. Comparison of the π–donating properties of an anionic BNC gold(I) complex among other complexes

Experimentally, complex **4-5tCl** and **4-5tLi** have a C–Au bond length of 2.050 and 2.017 Å. This slightly reduction of the bond length of product **4-5tLi** suggests that other type of interaction is involved between the BNC moiety and the gold atom. Indeed, NBO calculations show that there is an important donor-acceptor interaction between the filled *p*-orbital of carbon carbene and a vacant *p*-orbital of gold atom (p(C)→p(Au)) ($\mathbf{E_{C\rightarrow Au}}$) (**Figure 4-32**).

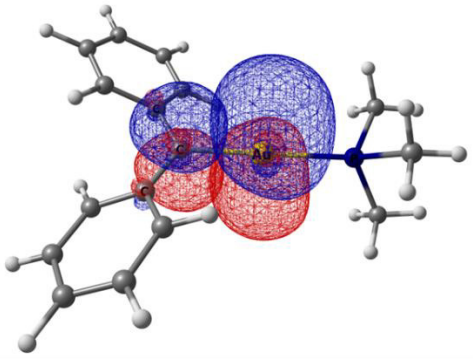
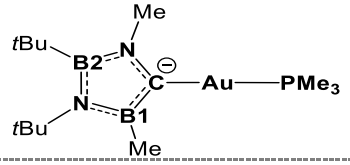
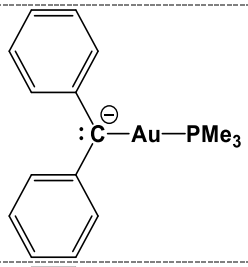
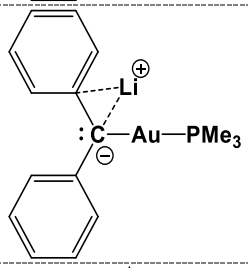
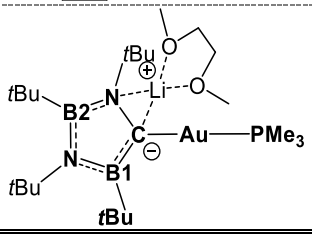


Figure 4-32. NBO donor-acceptor plot of the filled *p*-orbital of carbon carbene and a vacant *p*-orbital of gold atom of **$NPh_2CAuPMe_3$**.

In **Table 4-3** the complexes are given from the most π–donating to the lowest one according to their $E_{C\rightarrow Au}$ values and follows the order of: **$NBNCAuPMe_3$** (42.5 kcal/mol) > **$NPh_2CAuPMe_3$** (37.7 kcal/mol) > **$LiPh_2CAuPMe_3$** (18.3 kcal/mol) > **4-5tLi** (15.5 kcal/mol). Overall, the complex that does not contain lithium cationic delocalizes better the electron pair of the carbene towards gold atom. The introduction of the lithium cation reduces this interaction due to the interaction of the lone pair with lithium cation.

Table 4-3. Donor-acceptor interaction energies (kcal/mol) of p(C)→p(Au) ($E_{C\rightarrow Au}$).

	Structure	**$E_{C\rightarrow Au}$** (kcal/mol)
$NBNCAuPMe_3$		42.5

$NPh_2CAuPMe_3$		37.7
$LiPh_2CAuPMe_3$		18.3
4-5tLi		15.5

Moreover, NBO allows to re-optimize a molecule with a deleted donor-acceptor interaction, allowing to observe how the geometry parameters changes. However, till the date, it only works with small systems. Therefore, the simple system **$SBNCAuPMe_3$** was re-optimized with the deleted interaction p(C)→p(Au) (**Figure 4-33**). As expected, the C-Au bond increases from 1.963 to 1.981 Å an increase of 0.018 Å which is almost the half of the expected value of 0.033 Å for **AutLi**. Therefore, the π–donation factor alone is not enough to explain the overall C–Au bond length reduction. The other factor that maybe involved is the higher σ–donation of this new reduced BNC carbene (see appendix: **SFigure 1**) which may strength the C–Au bond.

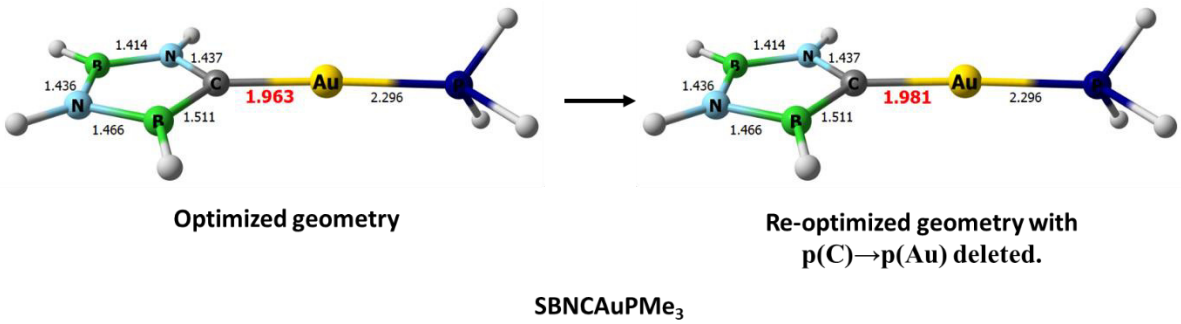


Figure 4-33. Re-optimization of **SBNCAuPMe3** with the deleted interaction p(C)→p(Au).

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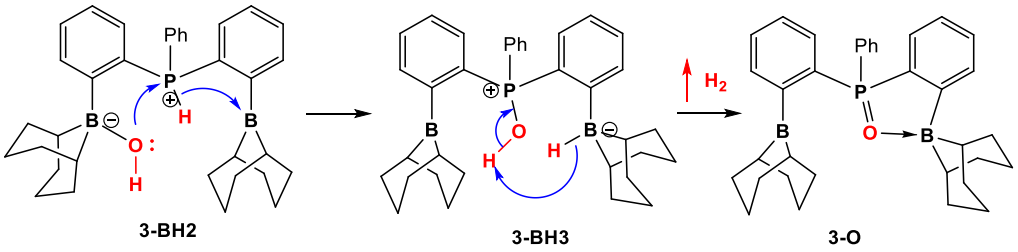
CONCLUSIONS

Conclusions of CHAPTER 3

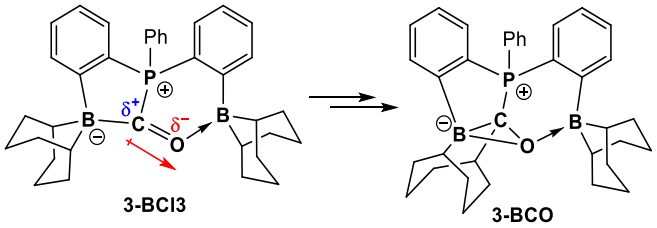
According to the presented theoretical calculations, the second borane in the diboro-phosphine FLP enhances the reactivity towards H_2O and CO compared with normal FLPs conformed by a phosphine and a borane.

1. For the diboro-phosphine FLP **3-BBN** that contains the 9-Borabicyclo[3.3.1]nonane ligands (9-BBN) the reaction with

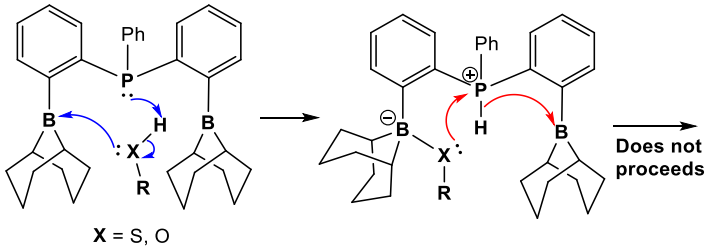
    - H_2O produces H_2 and the phosphine oxide **3-O**. The most important step of the reaction mechanism (**Figure 3-3**, between **3-BH2** and **3-BH3**) reveals that the hydroxyl group of borane attacks the phosphine and the hydrogen is displaced as hydride towards the second borane, showing the importance of this second borane. This hydride can then deprotonate the hydroxyl group of phosphine to generate phosphine oxide **3-O**.



    - CO produces compound **3-BCO**. The importance of the second borane comes from the fact that when oxygen coordinates with the second borane, the carbonyl group becomes more electrophilic, allowing to one of the substituents of the 9-BBN to migrate towards it.



    - Activation of H_2 is highly endergonic (22.1 kcal/mol) and the theoretical calculations show that is due to the low acidity of borane.
    - The rest of the molecules (MeOH, PhOH, *n*BuSH) showed an unfavored attack of the nucleophile towards the phosphorus atom that displaces the hydrogen as hydride towards borane (red arrows).



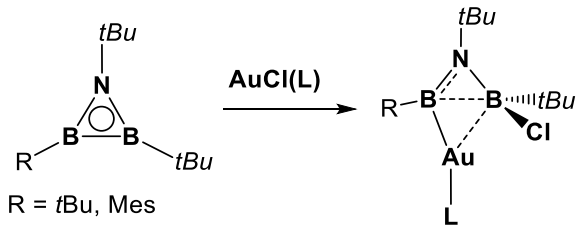
2. For the diboro-phosphine FLP **3-Cy**, which contains the cyclohexyl substituents at boron, the reaction mechanism with CO and H_2O is different than for the one observed in **3-BBN** because experimentally a different product is obtained; tricyclohexylborane is produced in both reactions.

    - Even though the reaction mechanism is not yet complete, the overall results that indicate that boranes in **3-Cy** are more acidic than the boranes in **3-BBN**, reflected in the lower energy barriers and intermediate energies of the calculated energetic profiles. Moreover, the total energy barrier for the reaction of **3-Cy** FLP with CO (+13.8 kcal/mol) indicates that the migration of the cyclohexyl of the boranes is much faster than borane substituents of **3-BBN** (18.7 kcal/mol). Therefore, the fully calculated reaction mechanisms may involve more Cy migrations.

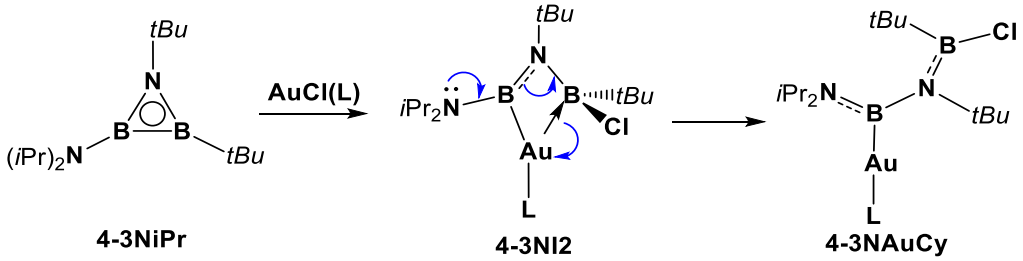
Conclusions of CHAPTER 4

1. Reaction of azadiboriridine with gold(I) complexes can lead to two products depending on the type of substituents in azadiboriridine:

    - Mesityl and tert-Butyl substituents in azadiboriridine generate the already reported azadiboriridine gold(I) complexes.[73]

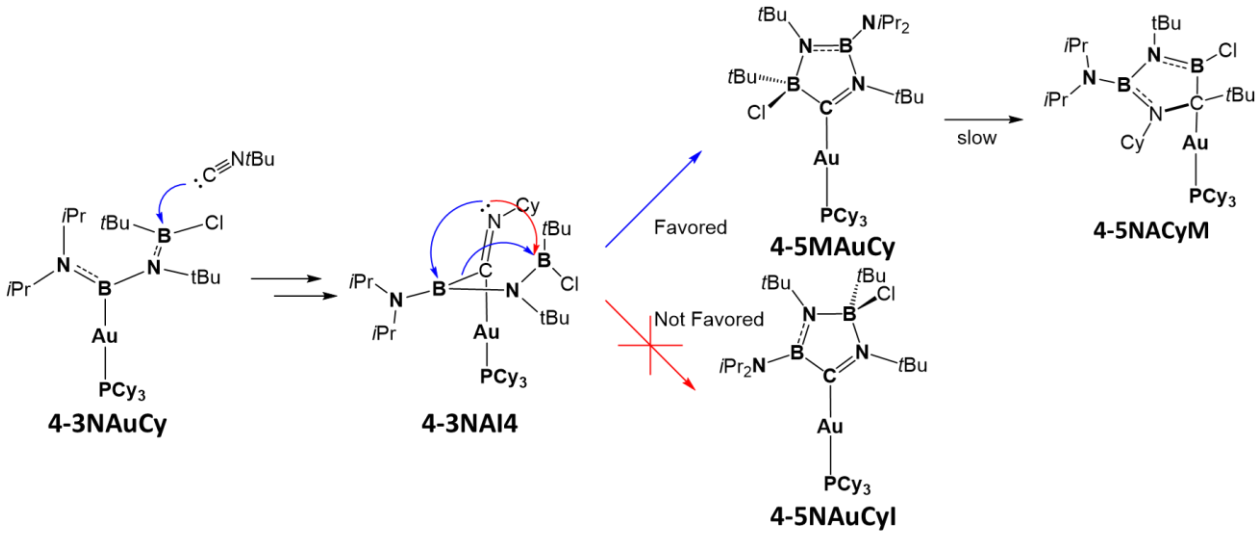


    - However, diisopropylamino substituent in the azadiboriridine does not produces the azadiboriridine gold(I) complex as a product. Instead, it is proposed to be an intermediate (**4-3NI2**). The electron lone pair of diisopropylamino substituent can stabilize the adjacent boron and thus, the other nitrogen stabilizes the other boron, decoordinating the borane from gold atom. This produces complex **4-3NAuCy**.



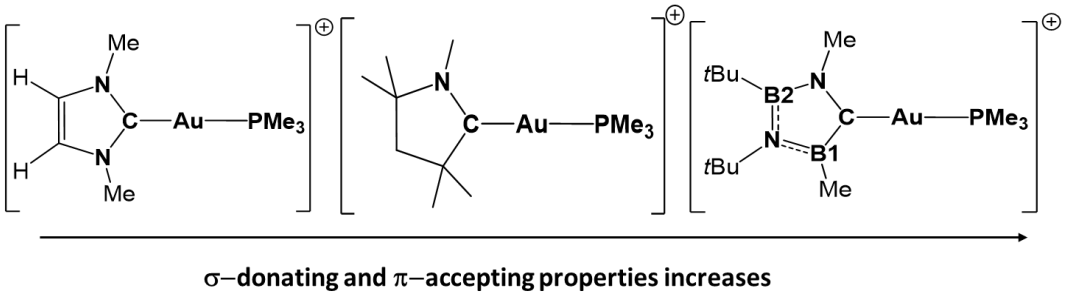
2. The azadiboriridine gold(I) complexes and complex **4-3NI2** further react with an isocyanide to produce the BNC carbene gold(I) complex.

- *tert*-butyl and mesityl azadiboriridine derivatives lead to similar structures already reported,[73] analogues to **4-5NAuCyI**.
- However, complex **4-3NAuCy** does not leads to the expected product 4-**5NAuCyI**, instead isomer **4-5NAuCy** is observed. The reaction mechanism reveals that when intermediate **4-3NAI4** is formed, migration of the carbon carbene is preferred (blue arrows) rather than the direct attack of nitrogen towards the borane (red arrows), generating **4-5MAuCy**. Then migration of the adjacent tBu group towards carbon carbene occurs slowly at room temperature (**4-5NAuCyM**).

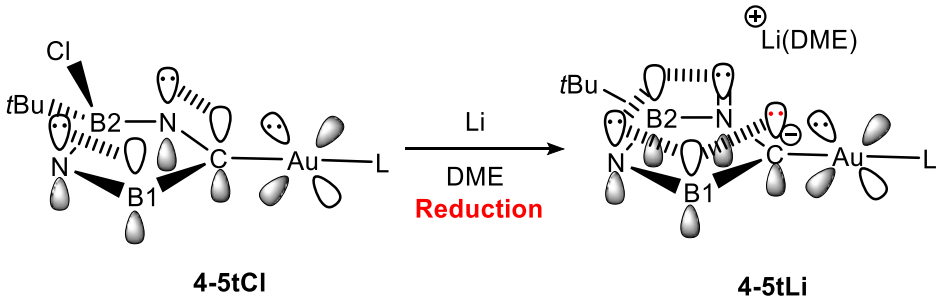


3. Natural Bond Orbital and Molecular Orbital calculations shows that BNC gold (I) complexes have better σ–donating and π–accepting properties than CAAC and NHC gold(I) complexes.

- According to NBO the adjacent electropositive boron atom allows carbon carbene to increase its σ–donating properties through charge transfer. The π–accepting properties also increases because the electron population in the *p*-orbital of carbon carbene is delocalized towards boron B1 and boron B2.



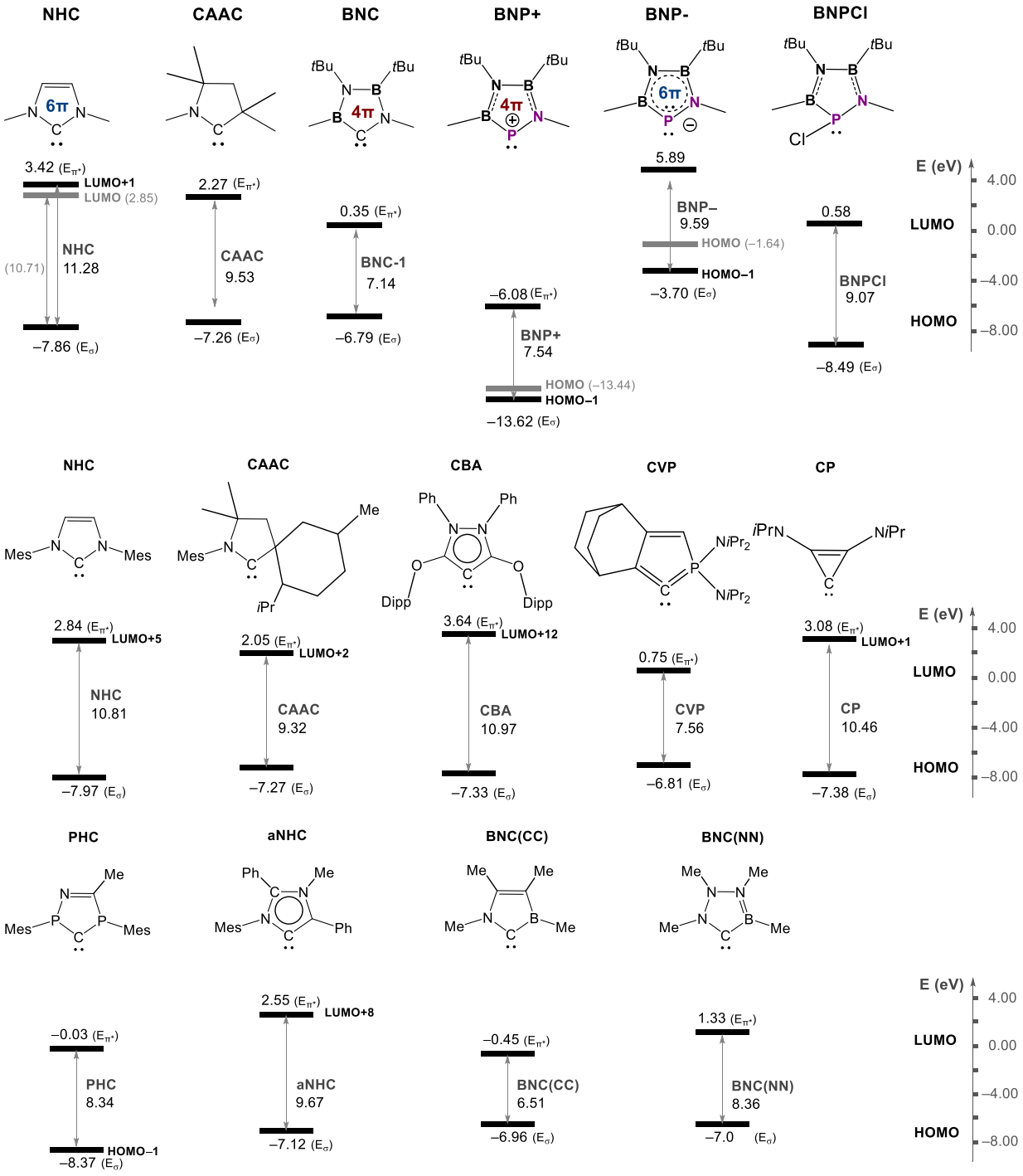
4. Reduction of a BNC gold(I) complex occurs at the BNC moiety and generates a 6π electron ring, which is calculated to be aromatic according to NICS and ACID calculations. According to NBO calculations, this reduced BNC carbene now behaves as a π–donor ligand.



4-5tCl **4-5tLi**

APPENDIX

π-accepting and σ-donating properties of diverse carbenes according to the MO energies



SFigure 1. E_σ and $E_{\pi*}$ energies (eV) of diverse carbenes.

Cartesian Coordinates (in x-y-z format)

3–BBN

SCF energy = –1711.26413491

5	–2.839071	–0.394710	–0.402613
5	2.305690	–0.851304	0.559485
15	–0.239752	0.854022	–0.227079
6	1.100829	2.033698	–0.660481
6	1.367859	2.240152	–2.016012
1	0.779861	1.716050	–2.763825
6	2.381598	3.100369	–2.416782
1	2.578256	3.248199	–3.473402
6	3.150023	3.759179	–1.464000
1	3.950593	4.422349	–1.774559
6	2.893560	3.561415	–0.112369
1	3.491847	4.072046	0.635077
6	1.874325	2.706235	0.288404
1	1.689669	2.549176	1.345647
6	–1.734438	1.889822	–0.043106
6	–2.928456	1.153459	–0.128045
6	–4.135803	1.832303	0.058713
1	–5.077845	1.292692	0.008408
6	–4.153903	3.203562	0.288094
1	–5.102696	3.715362	0.415721
6	–2.965059	3.922392	0.347059
1	–2.982960	4.993499	0.520112
6	–1.752824	3.263239	0.187651
1	–0.819588	3.815943	0.239002
6	0.195186	0.417112	1.504441
6	1.380360	–0.320249	1.708123
6	1.742221	–0.630233	3.023996
1	2.673013	–1.160073	3.209260
6	0.932166	–0.293277	4.102111
1	1.223472	–0.570238	5.110237
6	–0.241237	0.413094	3.882364
1	–0.876744	0.693293	4.716302
6	–0.595791	0.785124	2.590102
1	–1.499733	1.363102	2.430553
6	–2.977288	–1.047657	–1.824665
1	–2.871327	–0.319345	–2.636472
6	–1.921783	–2.153361	–2.030065
1	–2.121860	–2.687927	–2.967807
1	–0.956049	–1.654243	–2.166027
6	–1.792437	–3.177341	–0.888804
1	–0.838921	–3.705793	–1.002937
1	–2.558937	–3.947658	–0.998297
6	–1.855716	–2.583729	0.529161
1	–0.877331	–2.162417	0.785534
1	–2.025383	–3.393717	1.250205
6	–2.898690	–1.469774	0.744294
1	–2.735374	–1.041729	1.739282
6	–4.378037	–1.951152	0.692257
1	–4.530210	–2.730232	1.449232
1	–5.022550	–1.114386	0.995016
6	–4.842686	–2.464859	–0.678980
1	–4.448040	–3.467851	–0.847176
1	–5.932299	–2.578329	–0.665525
6	–4.450513	–1.550003	–1.849663
1	–5.110970	–0.671989	–1.849417
1	–4.641452	–2.063998	–2.799582
6	3.868182	–0.670993	0.550331
1	4.216842	0.024772	1.322664
6	4.497342	–2.058689	0.853520
1	5.583237	–2.009392	0.703365
1	4.354436	–2.263471	1.922384
6	3.918675	–3.240669	0.055742
1	4.385830	–3.295026	–0.928960
1	4.194034	–4.174188	0.558531
6	2.394073	–3.193440	–0.107308
1	1.919067	–3.445277	0.851084
1	2.075430	–3.972609	–0.810414
6	1.836446	–1.822578	–0.585042
1	0.751395	–1.926039	–0.645751
6	2.344295	–1.378197	–1.971749
1	2.188120	–2.184365	–2.700340
1	1.699718	–0.554447	–2.296878
6	3.808373	–0.908970	–2.035444
1	4.473141	–1.766682	–2.158016
1	3.944581	–0.307538	–2.940964
6	4.262066	–0.081744	–0.825152
1	3.833086	0.924023	–0.902482
1	5.350302	0.052748	–0.869126

3–BBN–H

SCF energy = –1712.42024893

5	–2.744337	–0.320572	–0.223314
5	2.515902	–0.967429	0.320608
15	–0.179110	0.823968	–0.004427
6	1.244159	1.981434	–0.200132
6	1.523553	2.467482	–1.478809

1	0.932452	2.133909	–2.327825
6	2.543713	3.386896	–1.679778
1	2.750748	3.755642	–2.678482
6	3.297770	3.830772	–0.598995
1	4.098519	4.546078	–0.753552
6	3.027393	3.354882	0.678244
1	3.616481	3.696515	1.522439
6	2.005196	2.434526	0.878171
1	1.805606	2.064792	1.878177
6	–1.608874	1.919846	0.112195
6	–2.844480	1.268410	–0.020971
6	–3.976339	2.093511	0.020742
1	–4.961618	1.653691	–0.092004
6	–3.868488	3.465113	0.204927
1	–4.767131	4.074314	0.238854
6	–2.622470	4.073979	0.345713
1	–2.547063	5.146191	0.491241
6	–1.475573	3.299686	0.290863
1	–0.500766	3.765458	0.384715
6	0.302369	–0.117626	1.473404
6	1.540914	–0.777364	1.534740
6	1.876967	–1.385442	2.749952
1	2.833779	–1.890565	2.844786
6	1.012979	–1.369771	3.838505
1	1.297166	–1.863981	4.761665
6	–0.208194	–0.716445	3.746305
1	–0.889663	–0.700293	4.589600
6	–0.560454	–0.079574	2.564073
1	–1.515586	0.428089	2.481328
6	–2.976274	–0.874288	–1.728796
1	–2.471322	–0.244004	–2.478423
6	–2.349250	–2.278110	–1.828104
1	–2.527926	–2.720873	–2.818570
1	–1.258909	–2.156342	–1.747980
6	–2.798454	–3.281601	–0.751182
1	–2.103024	–4.129968	–0.746898
1	–3.763528	–3.708933	–1.033150
6	–2.891209	–2.707156	0.673082
1	–1.876190	–2.626782	1.086161
1	–3.420354	–3.432092	1.308294
6	–3.540253	–1.313920	0.777049
1	–3.450670	–0.999422	1.827747
6	–5.044139	–1.298407	0.436949
1	–5.583723	–2.035146	1.049255
1	–5.447668	–0.323103	0.736935
6	–5.390249	–1.544821	–1.043118
1	–5.370149	–2.618070	–1.245770
1	–6.429454	–1.241966	–1.220219
6	–4.480981	–0.821888	–2.052307
1	–4.773940	0.235325	–2.100601
1	–4.677164	–1.229022	–3.054443
6	4.069587	–0.747170	0.386223
1	4.384038	–0.215922	1.292222
6	4.724052	–2.157057	0.420066
1	5.810912	–2.055089	0.312241
1	4.563839	–2.583616	1.418270
6	4.190485	–3.153679	–0.622611
1	4.675813	–2.988876	–1.585640
1	4.477077	–4.167385	–0.323155
6	2.668663	–3.104039	–0.803807
1	2.185058	–3.552001	0.074744
1	2.376345	–3.730501	–1.654176
6	2.082970	–1.673352	–1.013305
1	1.000593	–1.807234	–1.115891
6	2.613465	–0.956522	–2.271217
1	2.495702	–1.606744	–3.146680
1	1.963736	–0.094029	–2.457293
6	4.067496	–0.456508	–2.198115
1	4.751433	–1.257277	–2.485327
1	4.206598	0.323642	–2.954472
6	4.486505	0.107244	–0.833168
1	4.051755	1.104948	–0.711792
1	5.574047	0.251581	–0.824395
1	–1.508261	–0.501160	0.028079
1	–0.034103	0.166465	–1.230788

3–C6F5

SCF energy = –3995.88839804

5	2.043917	1.054892	1.466536
5	–1.376463	–0.196252	–1.457219
15	–1.047515	0.760395	1.203813
6	–2.743309	0.420282	1.808379
6	–2.993609	–0.870041	2.281006
1	–2.189605	–1.599600	2.299536
6	–4.267493	–1.228647	2.704950
1	–4.453589	–2.235689	3.063324
6	–5.302850	–0.302435	2.654836
1	–6.302130	–0.586537	2.967176
6	–5.061007	0.983880	2.185681
1	–5.870164	1.703735	2.130104
6	–3.787566	1.344591	1.763871
1	–3.614895	2.338794	1.365439
6	–0.244514	1.644086	2.599269

6	1.160438	1.632879	2.632841
6	1.810823	2.185426	3.736287
1	2.896310	2.167721	3.789533
6	1.092837	2.764495	4.775611
1	1.616809	3.191488	5.624233
6	–0.293534	2.777551	4.733150
1	–0.861327	3.216210	5.546828
6	–0.959010	2.204904	3.655367
1	–2.043390	2.179998	3.650422
6	–1.270382	1.987441	–0.129433
6	–1.318582	1.392166	–1.402132
6	–1.435903	2.225836	–2.516162
1	–1.473351	1.801591	–3.512572
6	–1.517611	3.604987	–2.362466
1	–1.594547	4.237435	–3.240645
6	–1.496954	4.178305	–1.096224
1	–1.559776	5.254725	–0.983014
6	–1.363478	3.367685	0.023211
1	–1.299001	3.807139	1.013864
6	2.809916	–0.293871	1.707435
6	2.210894	–1.363651	2.374091
6	4.121356	–0.498718	1.279387
6	2.843496	–2.583991	2.542798
6	4.789676	–1.694921	1.454092
6	4.138469	–2.747031	2.081760
6	2.160760	1.852525	0.119715
6	1.824408	3.207937	0.031389
6	2.476400	1.244307	–1.099651
6	1.755720	3.891932	–1.169012
6	2.390568	1.890416	–2.317092
6	2.010115	3.222003	–2.351868
6	–0.078240	–1.052680	–1.785226
6	0.498963	–0.940261	–3.041395
6	0.511780	–1.975739	–0.927836
6	1.593082	–1.686498	–3.446490
6	1.617602	–2.722682	–1.289107
6	2.159568	–2.581108	–2.556070
6	–2.773974	–0.901240	–1.279361
6	–3.961872	–0.166533	–1.124021
6	–2.927299	–2.289152	–1.140769
6	–5.170857	–0.741573	–0.777110
6	–4.118929	–2.889774	–0.777140
6	–5.244698	–2.108389	–0.580087
9	0.014080	–2.196496	0.290186
9	2.164186	–3.581099	–0.429683
9	3.218491	–3.295388	–2.909500
9	2.100872	–1.544942	–4.664182
9	–0.038616	–0.099391	–3.938129
9	–1.911494	–3.122041	–1.346060
9	–4.194241	–4.206750	–0.620043
9	–6.386100	–2.666030	–0.217103
9	–6.256687	0.006733	–0.621131
9	–3.991477	1.149458	–1.296247
9	4.790729	0.492245	0.686489
9	6.040136	–1.847735	1.033735
9	4.758954	–3.903046	2.244910
9	2.223689	–3.591053	3.144722
9	0.974362	–1.265410	2.853009
9	1.549223	3.918052	1.120440
9	1.421412	5.176725	–1.197295
9	1.904092	3.852717	–3.507293
9	2.670437	1.253683	–3.448936
9	2.864943	–0.028492	–1.141984

3–C6F5–H

SCF energy = –3997.07547522

5	2.065556	–0.473452	–0.838002
5	–1.975929	0.177176	1.416248
15	–0.946414	–0.810236	–1.413178
6	–2.628392	–0.914189	–2.059387
6	–3.276236	0.260537	–2.445118
1	–2.760657	1.213630	–2.399556
6	–4.598081	0.210556	–2.868410
1	–5.104206	1.124036	–3.160031
6	–5.269293	–1.005664	–2.907905
1	–6.306601	–1.041195	–3.222308
6	–4.620886	–2.177633	–2.532517
1	–5.150678	–3.122868	–2.550454
6	–3.302185	–2.134941	–2.105759
1	–2.810855	–3.044209	–1.775176
6	0.277556	–1.241029	–2.638584
6	1.621674	–1.010751	–2.304612
6	2.545523	–1.243694	–3.328881
1	3.598200	–1.067879	–3.128593
6	2.160767	–1.706106	–4.576823
1	2.912200	–1.883859	–5.339687
6	0.818229	–1.946509	–4.864615
1	0.520352	–2.308117	–5.842539
6	–0.136238	–1.703026	–3.894618
1	–1.187631	–1.857838	–4.114261
6	–0.860000	–1.780508	0.100728
6	–1.344731	–1.265781	1.315194
6	–1.237483	–2.077360	2.443475

1	–1.584249	–1.710824	3.403815
6	–0.676112	–3.346576	2.369464
1	–0.587521	–3.945515	3.269248
6	–0.223716	–3.845164	1.157310
1	0.226301	–4.829492	1.098027
6	–0.313360	–3.058390	0.017868
1	0.084304	–3.423338	–0.923714
6	3.018331	0.837132	–0.992420
6	2.447889	2.019894	–1.444393
6	4.368382	0.917464	–0.690402
6	3.133089	3.216180	–1.558355
6	5.099194	2.094542	–0.786894
6	4.476807	3.252074	–1.219366
6	2.615552	–1.630177	0.172939
6	2.831557	–2.966746	–0.123825
6	2.756877	–1.313882	1.519035
6	3.127764	–3.927286	0.833254
6	3.038608	–2.235449	2.510488
6	3.224531	–3.563495	2.162126
6	–0.963973	1.380708	1.511835
6	0.071729	1.375735	2.441255
6	–0.955856	2.434136	0.602911
6	1.057736	2.346734	2.469223
6	0.020644	3.408335	0.580927
6	1.040262	3.355572	1.519900
6	–3.517981	0.368775	1.268526
6	–4.362820	–0.687480	0.888393
6	–4.146900	1.616005	1.404796
6	–5.696975	–0.506304	0.572572
6	–5.479327	1.825292	1.100963
6	–6.253110	0.758314	0.669091
9	–1.900248	2.494752	–0.354238
9	–0.002907	4.375619	–0.322215
9	1.988651	4.276335	1.513298
9	2.012243	2.319590	3.384320
9	0.113676	0.426284	3.375875
9	–3.476458	2.670354	1.849778
9	–6.025866	3.026773	1.225355
9	–7.523975	0.944317	0.367388
9	–6.449884	–1.529107	0.185942
9	–3.914862	–1.933269	0.801502
9	5.040917	–0.168724	–0.283103
9	6.393704	2.119698	–0.474020
9	5.162741	4.387190	–1.321530
9	2.527674	4.320487	–1.992154
9	1.141620	2.040944	–1.794335
9	2.695520	–3.431680	–1.379282
9	3.266233	–5.210179	0.485850
9	3.479919	–4.477287	3.096754
9	3.129774	–1.865577	3.787162
9	2.599703	–0.041712	1.916188
1	–0.829231	0.540069	–1.094182
1	1.070491	–0.050017	–0.267279

H2

SCF energy = –1.17311664788

1	0.000000	0.000000	0.370988
1	0.000000	0.000000	–0.370988

3–BH1

SCF energy = –1787.69042769

5	2.618637	–0.591681	–0.596743
8	1.262198	–1.333658	–1.384300
5	–2.548082	–0.971871	–0.492321
15	–0.257964	0.897966	–0.032689
6	–0.790886	1.854781	1.433281
6	–2.003212	2.539938	1.492856
1	–2.664774	2.547987	0.632823
6	–2.372142	3.212859	2.652851
1	–3.318592	3.742457	2.687487
6	–1.534425	3.209175	3.760199
1	–1.823623	3.734498	4.664370
6	–0.321167	2.530913	3.705044
1	0.340923	2.526746	4.564552
6	0.048120	1.855498	2.551089
1	1.001951	1.337453	2.514874
6	1.288798	1.752151	–0.538654
6	2.425040	0.996164	–0.912237
6	3.486751	1.725667	–1.466832
1	4.359319	1.193052	–1.826156
6	3.479829	3.110548	–1.568240
1	4.333933	3.624774	–1.998065
6	2.393528	3.834544	–1.096483
1	2.391842	4.919230	–1.130582
6	1.299070	3.149691	–0.591812
1	0.444427	3.707855	–0.221005
6	–1.522298	1.278650	–1.311237
6	–2.546304	0.315311	–1.405712
6	–3.554797	0.518721	–2.354072
1	–4.353934	–0.209614	–2.456962
6	–3.551817	1.633136	–3.183903
1	–4.345313	1.767379	–3.912192

6	–2.519259	2.557842	–3.100654
1	–2.497795	3.415650	–3.764754
6	–1.504741	2.377108	–2.168903
1	–0.690164	3.090500	–2.125107
6	2.445601	–1.028132	0.947809
1	1.565500	–0.570254	1.418345
6	2.254345	–2.553508	1.071817
1	2.282319	–2.848933	2.129491
1	1.240292	–2.790617	0.731681
6	3.247536	–3.429821	0.284793
1	2.815040	–4.429959	0.166967
1	4.151639	–3.580363	0.878336
6	3.643172	–2.894788	–1.102430
1	2.847652	–3.137715	–1.814242
1	4.530926	–3.441656	–1.446646
6	3.909758	–1.375409	–1.159998
1	4.129117	–1.130280	–2.211269
6	5.164462	–0.977241	–0.340473
1	6.009324	–1.613138	–0.636491
1	5.458006	0.042040	–0.608845
6	5.014250	–1.028380	1.190253
1	5.150580	–2.050701	1.548331
1	5.830724	–0.454124	1.642604
6	3.674381	–0.487390	1.704149
1	3.675951	0.607759	1.619168
1	3.586027	–0.710059	2.775758
6	–2.915558	–0.983837	1.035188
1	–2.904823	0.007811	1.495963
6	–4.402651	–1.448003	1.022776
1	–4.772387	–1.496374	2.053886
1	–4.998631	–0.668118	0.529089
6	–4.658735	–2.788429	0.319993
1	–4.355649	–3.608628	0.971560
1	–5.737441	–2.914983	0.177478
6	–3.962985	–2.918230	–1.043854
1	–4.535855	–2.347836	–1.785744
1	–4.002795	–3.961172	–1.380919
6	–2.482404	–2.431904	–1.081280
1	–2.166144	–2.457601	–2.130995
6	–1.525858	–3.327954	–0.266599
1	–1.613249	–4.365704	–0.612640
1	–0.498994	–3.031113	–0.505187
6	–1.715780	–3.290223	1.258094
1	–2.529840	–3.960175	1.541652
1	–0.821747	–3.711985	1.729659
6	–1.962874	–1.889901	1.841836
1	–1.001676	–1.367437	1.917017
1	–2.329675	–1.989340	2.870878
1	0.494424	–0.994354	–0.871962
1	1.181787	–1.002695	–2.284079

3–BH2

SCF energy = –1787.69365706

5	–2.328125	–0.586221	0.230377
8	–0.823040	–0.709604	0.602833
5	2.223771	–1.291674	0.416105
15	0.129072	1.192701	–0.043341
6	1.029261	2.555517	–0.897395
6	2.219744	3.103870	–0.426210
1	2.639254	2.770232	0.516277
6	2.885076	4.079077	–1.163051
1	3.810484	4.499937	–0.784421
6	2.368652	4.509411	–2.376688
1	2.888244	5.269707	–2.950300
6	1.184493	3.960220	–2.859941
1	0.777321	4.290897	–3.809396
6	0.521704	2.988247	–2.126380
1	–0.405825	2.568922	–2.507685
6	–1.505965	1.886391	0.295324
6	–2.597593	1.011659	0.446356
6	–3.825925	1.632266	0.711792
1	–4.714039	1.022192	0.817568
6	–3.954861	3.007118	0.847989
1	–4.928473	3.436884	1.064243
6	–2.849886	3.839967	0.705977
1	–2.947685	4.914978	0.811619
6	–1.619792	3.276800	0.414301
1	–0.757942	3.920884	0.274369
6	1.146791	0.887738	1.429081
6	1.996332	–0.224495	1.545012
6	2.682095	–0.375856	2.756443
1	3.325502	–1.239704	2.893969
6	2.562859	0.544726	3.790089
1	3.117904	0.401586	4.711238
6	1.707736	1.628763	3.653358
1	1.586610	2.340966	4.462292
6	0.988028	1.792332	2.476769
1	0.295277	2.623015	2.385543
6	–2.539733	–1.015402	–1.327848
1	–2.006001	–0.337413	–2.016163
6	–1.955564	–2.421455	–1.553215
1	–2.155034	–2.766578	–2.578200
1	–0.869843	–2.331587	–1.471558

6	–2.415343	–3.509754	–0.566384
1	–1.721104	–4.357443	–0.630216
1	–3.380336	–3.911988	–0.882865
6	–2.513552	–3.055309	0.899483
1	–1.503497	–3.031269	1.327116
1	–3.055937	–3.822883	1.469036
6	–3.173841	–1.674004	1.101086
1	–3.128106	–1.451794	2.180459
6	–4.667704	–1.698374	0.717785
1	–5.159431	–2.559921	1.191489
1	–5.156487	–0.823233	1.157227
6	–4.971210	–1.736263	–0.793991
1	–4.945766	–2.770889	–1.143227
1	–6.004734	–1.407417	–0.956520
6	–4.034228	–0.891908	–1.673550
1	–4.317830	0.164597	–1.587075
1	–4.209771	–1.160752	–2.724419
6	2.631216	–0.949164	–1.062657
1	2.511888	0.106521	–1.333321
6	4.168542	–1.206206	–1.035234
1	4.588773	–0.941358	–2.012320
1	4.625612	–0.512270	–0.315970
6	4.568813	–2.641324	–0.674434
1	4.368376	–3.297290	–1.522510
1	5.653263	–2.681025	–0.525562
6	3.873808	–3.177231	0.587416
1	4.392360	–2.768475	1.464526
1	4.001932	–4.264890	0.647428
6	2.364722	–2.827139	0.714021
1	2.052620	–3.090808	1.731664
6	1.450490	–3.591331	–0.268700
1	1.544756	–4.670370	–0.095649
1	0.413954	–3.334244	–0.027100
6	1.706773	–3.297697	–1.753321
1	2.582062	–3.857275	–2.089078
1	0.869674	–3.696701	–2.335384
6	1.871935	–1.805774	–2.097601
1	0.872947	–1.371314	–2.219431
1	2.353184	–1.710262	–3.078926
1	0.201377	0.261505	–1.072765
1	–0.758768	–0.880379	1.544934

3–BH3

SCF energy = –1787.67913572

5	–2.508590	–0.646469	–0.090771
8	–0.759598	–0.402477	–0.417179
5	2.363421	–0.527790	0.294306
15	–0.032940	0.991095	0.121948
6	0.646706	2.041526	–1.181529
6	–0.077881	2.199023	–2.361183
1	–1.041833	1.714424	–2.480958
6	0.442932	2.981292	–3.382689
1	–0.110668	3.097413	–4.307893
6	1.668324	3.617330	–3.217450
1	2.070198	4.231174	–4.016436
6	2.378272	3.471576	–2.031342
1	3.333389	3.968273	–1.901929
6	1.874690	2.676155	–1.011945
1	2.435228	2.540392	–0.093964
6	–1.660034	1.729466	0.424506
6	–2.766763	0.875199	0.330545
6	–4.020926	1.445837	0.585656
1	–4.913979	0.832689	0.535766
6	–4.156223	2.790388	0.899328
1	–5.143013	3.201038	1.088902
6	–3.040780	3.622876	0.955634
1	–3.153286	4.678075	1.179678
6	–1.786686	3.089746	0.712193
1	–0.909683	3.731281	0.737814
6	0.855637	0.966253	1.683093
6	2.070702	0.262991	1.655108
6	2.825094	0.287347	2.834410
1	3.777443	–0.230629	2.873441
6	2.370563	0.945372	3.968565
1	2.974172	0.938176	4.871338
6	1.140425	1.601788	3.973078
1	0.785861	2.097329	4.870112
6	0.369182	1.614824	2.823850
1	–0.592624	2.114115	2.817580
6	–3.100771	–1.208595	–1.467790
1	–3.043411	–0.466352	–2.275740
6	–2.310240	–2.451880	–1.921938
1	–2.771509	–2.883967	–2.819198
1	–1.312949	–2.127322	–2.249288
6	–2.162579	–3.558477	–0.863456
1	–1.375151	–4.250815	–1.181545
1	–3.075816	–4.156277	–0.842431
6	–1.841740	–3.063636	0.558659
1	–0.764143	–2.870692	0.631730
1	–2.021801	–3.882803	1.266387
6	–2.591136	–1.796079	1.017439
1	–2.150784	–1.480429	1.972884
6	–4.099055	–2.028205	1.267112

1	–4.235576	–2.831320	2.002428
1	–4.509500	–1.127309	1.739026
6	–4.921778	–2.360947	0.009151
1	–4.788359	–3.415949	–0.237462
1	–5.987033	–2.255795	0.243972
6	–4.600956	–1.498801	–1.227603
1	–5.121470	–0.538556	–1.138621
1	–5.032048	–1.979496	–2.115173
6	3.707160	–0.277063	–0.561929
1	3.957917	0.789545	–0.639849
6	4.897644	–0.957801	0.144501
1	5.806097	–0.868560	–0.467178
1	5.109770	–0.394308	1.062067
6	4.694001	–2.439039	0.510344
1	4.888628	–3.061573	–0.365759
1	5.456659	–2.732405	1.241193
6	3.306587	–2.778070	1.079369
1	3.261056	–2.454736	2.126793
1	3.190750	–3.870122	1.103638
6	2.118494	–2.131492	0.340463
1	1.223612	–2.396106	0.923105
6	1.918754	–2.664775	–1.091201
1	1.836411	–3.760014	–1.090947
1	0.943292	–2.317246	–1.474890
6	2.991402	–2.239940	–2.109824
1	3.854469	–2.902038	–2.015570
1	2.607342	–2.415705	–3.121243
6	3.454803	–0.777342	–1.997093
1	2.688856	–0.127434	–2.442485
1	4.353519	–0.650014	–2.616002
1	1.394411	–0.036038	–0.415669
1	–0.160660	–1.146288	–0.563280

3–BH4

SCF energy = –1787.68115332

5	–2.673940	–0.588703	–0.459645
8	–0.339676	0.091784	–1.121631
5	1.946701	–1.311974	0.077765
15	–0.181114	1.185338	0.011130
6	0.898695	2.536390	–0.472423
6	1.890652	2.987377	0.395817
1	2.036652	2.500808	1.354004
6	2.712183	4.037702	0.008956
1	3.492521	4.383864	0.677143
6	2.544487	4.627464	–1.237594
1	3.195419	5.440315	–1.541499
6	1.552219	4.176157	–2.103209
1	1.428660	4.635992	–3.077308
6	0.722743	3.133301	–1.721995
1	–0.046351	2.772191	–2.397038
6	–1.844317	1.837581	0.131849
6	–2.896574	0.946881	–0.141526
6	–4.191834	1.471557	–0.062053
1	–5.042965	0.832275	–0.272093
6	–4.422957	2.797121	0.283357
1	–5.442039	3.166060	0.340016
6	–3.362327	3.656493	0.543826
1	–3.543446	4.694817	0.797794
6	–2.065114	3.176248	0.455568
1	–1.226387	3.843560	0.627993
6	0.362454	0.387932	1.512266
6	1.241954	–0.720359	1.447787
6	1.445460	–1.350216	2.686318
1	2.058593	–2.242210	2.717843
6	0.885726	–0.903378	3.874857
1	1.089759	–1.439357	4.797006
6	0.058704	0.214053	3.895616
1	–0.383687	0.566015	4.820961
6	–0.219967	0.849120	2.700245
1	–0.912451	1.685725	2.687213
6	–3.089021	–1.289594	–1.803127
1	–3.148953	–0.593264	–2.646880
6	–2.075081	–2.396513	–2.160549
1	–2.416572	–2.927290	–3.058165
1	–1.134573	–1.913505	–2.443833
6	–1.805046	–3.423279	–1.049944
1	–0.899801	–3.982709	–1.308016
1	–2.608059	–4.163748	–1.044282
6	–1.620507	–2.831682	0.360043
1	–0.579251	–2.525412	0.476366
1	–1.775683	–3.624239	1.103239
6	–2.501502	–1.619681	0.714845
1	–2.118331	–1.175805	1.640037
6	–3.994296	–1.993602	0.977189
1	–4.036304	–2.691168	1.821531
1	–4.536178	–1.096995	1.306576
6	–4.712419	–2.611660	–0.231404
1	–4.371475	–3.639537	–0.361295
1	–5.783086	–2.686166	–0.011642
6	–4.527215	–1.829900	–1.545148
1	–5.220846	–0.980063	–1.552043
1	–4.830349	–2.459772	–2.390343
6	2.869973	–0.262183	–0.771710

1	2.378182	0.690382	–0.996349
6	4.114649	0.104260	0.053111
1	4.733619	0.838170	–0.482997
1	3.775898	0.607842	0.970424
6	4.992892	–1.089931	0.448255
1	5.590592	–1.396158	–0.413175
1	5.721733	–0.766586	1.201315
6	4.207168	–2.292567	0.999915
1	3.987627	–2.083906	2.053279
1	4.869232	–3.170426	1.008865
6	2.886901	–2.629693	0.271209
1	2.381483	–3.404373	0.868469
6	3.120254	–3.252573	–1.117867
1	3.748287	–4.151685	–1.040872
1	2.148603	–3.592467	–1.499151
6	3.751284	–2.303877	–2.149677
1	4.830580	–2.260050	–1.986230
1	3.633438	–2.735869	–3.150874
6	3.173707	–0.878062	–2.152978
1	2.228941	–0.891213	–2.713543
1	3.849851	–0.226015	–2.724815
1	1.009861	–1.721485	–0.671462
1	0.313987	–0.692812	–1.009639

3–BO

SCF energy = –1786.54018391

5	–2.454998	0.587365	–0.160344
8	–0.827283	0.460637	–0.133231
5	2.670267	0.201101	–0.598033
15	–0.300450	–0.976586	0.013901
6	0.652005	–1.128435	1.540791
6	0.334684	–0.273764	2.598136
1	–0.409594	0.503015	2.456196
6	0.973880	–0.422382	3.820491
1	0.732674	0.247794	4.638024
6	1.919422	–1.427788	3.994348
1	2.417420	–1.542037	4.951226
6	2.234306	–2.282412	2.944125
1	2.979250	–3.059033	3.077745
6	1.605054	–2.133149	1.715205
1	1.866427	–2.789263	0.891247
6	–1.824956	–1.892014	0.093616
6	–2.883209	–0.976278	–0.020784
6	–4.169046	–1.536237	0.035606
1	–5.040242	–0.896903	–0.051265
6	–4.359258	–2.899356	0.206662
1	–5.369010	–3.296649	0.248718
6	–3.276639	–3.771959	0.335071
1	–3.442285	–4.833977	0.479976
6	–1.991346	–3.264182	0.280836
1	–1.133197	–3.922952	0.383250
6	0.785884	–1.531158	–1.316864
6	2.092405	–1.009115	–1.426380
6	2.904026	–1.535136	–2.435764
1	3.923059	–1.176238	–2.542908
6	2.437301	–2.498832	–3.324247
1	3.092530	–2.873616	–4.103925
6	1.144059	–2.984450	–3.210023
1	0.774447	–3.734848	–3.900071
6	0.321533	–2.508073	–2.196186
1	–0.686580	–2.895302	–2.095109
6	–2.870353	1.554007	1.069206
1	–2.644627	1.090304	2.042858
6	–2.050318	2.855136	0.980253
1	–2.352832	3.554253	1.772743
1	–1.001538	2.607274	1.177923
6	–2.124451	3.582202	–0.373909
1	–1.315304	4.320977	–0.422434
1	–3.045874	4.167755	–0.421258
6	–2.033401	2.664790	–1.606748
1	–0.983592	2.390611	–1.757993
1	–2.327007	3.240534	–2.495925
6	–2.847587	1.358417	–1.522153
1	–2.589573	0.761234	–2.409566
6	–4.372464	1.578058	–1.554359
1	–4.653209	2.163266	–2.440971
1	–4.853918	0.601638	–1.689235
6	–4.963991	2.263998	–0.308649
1	–4.822659	3.343384	–0.393957
1	–6.051326	2.119633	–0.305543
6	–4.394575	1.782071	1.039191
1	–4.884213	0.841687	1.318878
1	–4.684811	2.501464	1.817317
6	4.057103	0.195090	0.141573
1	4.472351	–0.811649	0.271300
6	5.037069	0.987985	–0.772229
1	5.983744	1.138814	–0.238903
1	5.285307	0.359647	–1.636903
6	4.512039	2.338948	–1.287186
1	4.648246	3.108163	–0.526048
1	5.129079	2.656910	–2.134608
6	3.041693	2.309268	–1.724451
1	2.960395	1.777549	–2.682464

1	2.695435	3.329939	–1.923446
6	2.068145	1.643358	–0.704317
1	1.071440	1.667207	–1.149284
6	1.993404	2.353349	0.660788
1	1.766040	3.416222	0.512509
1	1.126801	1.938016	1.182006
6	3.230662	2.214550	1.562844
1	3.975094	2.968414	1.299456
1	2.941177	2.445970	2.593851
6	3.879588	0.823025	1.543217
1	3.269089	0.142287	2.144147
1	4.854043	0.872686	2.045415

3–BOI

SCF energy = –1786.54018330

5	–2.454837	–0.587459	–0.160003
8	–0.827150	–0.460524	–0.132139
5	2.669977	–0.201039	–0.598240
15	–0.300461	0.976805	0.014286
6	0.652267	1.129004	1.540903
6	1.605604	2.133519	1.714884
1	1.867101	2.789271	0.890688
6	2.234998	2.282994	2.943708
1	2.980173	3.059434	3.077007
6	1.919971	1.428784	3.994225
1	2.418056	1.543194	4.951027
6	0.974126	0.423588	3.820784
1	0.732832	–0.246252	4.638555
6	0.334788	0.274753	2.598541
1	–0.409672	–0.501878	2.456848
6	–1.825104	1.892056	0.093751
6	–2.883222	0.976188	–0.020911
6	–4.169145	1.536000	0.034873
1	–5.040216	0.896544	–0.052266
6	–4.359582	2.899119	0.205698
1	–5.369385	3.296304	0.247292
6	–3.277114	3.771850	0.334474
1	–3.442929	4.833852	0.479238
6	–1.991737	3.264222	0.280755
1	–1.133714	3.923102	0.383418
6	0.785506	1.531111	–1.316931
6	2.092042	1.009095	–1.426672
6	2.903381	1.534872	–2.436395
1	3.922357	1.175916	–2.543744
6	2.436413	2.498404	–3.324949
1	3.091422	2.873050	–4.104864
6	1.143213	2.984030	–3.210466
1	0.773404	3.734285	–3.900548
6	0.320937	2.507840	–2.196324
1	–0.687139	2.895085	–2.095100
6	–2.870433	–1.553911	1.069628
1	–2.645140	–1.089897	2.043240
6	–2.049928	–2.854767	0.981262
1	–2.352442	–3.553762	1.773860
1	–1.001294	–2.606444	1.179193
6	–2.123393	–3.582222	–0.372722
1	–1.314019	–4.320789	–0.420764
1	–3.044663	–4.168025	–0.420282
6	–2.032170	–2.665112	–1.605778
1	–0.982381	–2.390732	–1.756796
1	–2.325406	–3.241128	–2.494911
6	–2.846680	–1.358911	–1.521769
1	–2.588512	–0.761879	–2.409233
6	–4.371493	–1.578949	–1.554460
1	–4.651784	–2.164312	–2.441126
1	–4.853135	–0.602652	–1.689561
6	–4.963246	–2.264929	–0.308886
1	–4.821441	–3.344288	–0.393911
1	–6.050647	–2.120993	–0.306288
6	–4.394559	–1.782534	1.039092
1	–4.884670	–0.842301	1.318467
1	–4.684776	–2.501931	1.817224
6	4.056856	–0.195122	0.141307
1	4.472281	0.811563	0.270885
6	5.036565	–0.988115	–0.772807
1	5.983468	–1.138650	–0.239784
1	5.284376	–0.359937	–1.637723
6	4.511557	–2.339223	–1.287301
1	4.647899	–3.108244	–0.525980
1	5.128512	–2.657353	–2.134729
6	3.041169	–2.309608	–1.724385
1	2.959814	–1.778182	–2.682557
1	2.694727	–3.330293	–1.922991
6	2.067778	–1.643239	–0.704369
1	1.071078	–1.667018	–1.149340
6	1.992826	–2.352836	0.660925
1	1.764925	–3.415638	0.512927
1	1.126473	–1.936915	1.182115
6	3.230252	–2.214419	1.562788
1	3.974347	–2.968628	1.299407
1	2.940805	–2.445621	2.593861
6	3.879782	–0.823159	1.542927
1	3.269908	–0.142225	2.144266

1	4.854479	–0.873272	2.044629

3–BOR

SCF energy = –1786.53520256

5	–2.624990	0.239441	–0.410513
8	0.503936	–0.118584	–0.845281
5	1.268571	–1.374848	–0.072204
15	0.510516	1.112243	0.090547
6	2.037187	2.062108	–0.094377
6	2.457465	2.400448	–1.381780
1	1.859710	2.114906	–2.241307
6	3.650718	3.083148	–1.561450
1	3.983780	3.332999	–2.562775
6	4.423070	3.434905	–0.458906
1	5.360021	3.962699	–0.601953
6	4.005207	3.100742	0.823054
1	4.613392	3.365577	1.681055
6	2.814201	2.409462	1.008067
1	2.504777	2.119203	2.006647
6	–0.852143	2.240724	–0.240823
6	–2.146146	1.740660	–0.482947
6	–3.146146	2.684711	–0.750617
1	–4.154399	2.346248	–0.964740
6	–2.895953	4.050595	–0.739352
1	–3.703461	4.747452	–0.939510
6	–1.616251	4.521957	–0.487475
1	–1.408673	5.586247	–0.486845
6	–0.594174	3.614574	–0.253540
1	0.411502	3.982821	–0.085730
6	0.475173	0.316148	1.680415
6	0.880869	–1.012731	1.474105
6	0.936242	–1.806332	2.627124
1	1.248622	–2.842075	2.556256
6	0.581824	–1.299747	3.870938
1	0.619724	–1.949137	4.740474
6	0.170778	0.024610	4.025959
1	–0.110802	0.400715	5.003580
6	0.122069	0.851273	2.915490
1	–0.204880	1.883743	3.004355
6	–3.328188	–0.495753	–1.608345
1	–3.143762	–0.012165	–2.574091
6	–2.797297	–1.942696	–1.681647
1	–3.285187	–2.470361	–2.510673
1	–1.733353	–1.900387	–1.933296
6	–2.982101	–2.749936	–0.390865
1	–2.408017	–3.678990	–0.472009
1	–4.024516	–3.066152	–0.309918
6	–2.544788	–2.014117	0.888838
1	–1.463803	–2.121616	1.001448
1	–2.984538	–2.512337	1.762380
6	–2.853966	–0.505355	0.949428
1	–2.302077	–0.074447	1.789681
6	–4.363755	–0.187028	1.189125
1	–4.654887	–0.595996	2.163499
1	–4.492115	0.900666	1.274235
6	–5.304051	–0.731453	0.105566
1	–5.412456	–1.808433	0.238301
1	–6.305920	–0.317638	0.264356
6	–4.861008	–0.416491	–1.336178
1	–5.203686	0.592166	–1.595170
1	–5.380250	–1.086424	–2.032355
6	2.866490	–1.278344	–0.354030
1	3.310921	–0.365268	0.067087
6	3.541535	–2.456277	0.376853
1	4.624891	–2.443151	0.195165
1	3.422991	–2.295676	1.455874
6	3.000751	–3.850422	0.016035
1	3.457665	–4.179798	–0.919405
1	3.344302	–4.571058	0.768020
6	1.467542	–3.946216	–0.103864
1	1.037834	–4.083058	0.895555
1	1.216241	–4.866616	–0.649021
6	0.766249	–2.739930	–0.762465
1	–0.307631	–2.898264	–0.624908
6	1.012213	–2.647330	–2.280827
1	0.678058	–3.569902	–2.775774
1	0.381993	–1.843079	–2.677159
6	2.466801	–2.364430	–2.683289
1	3.052938	–3.282882	–2.602934
1	2.497395	–2.098570	–3.746850
6	3.136140	–1.244760	–1.869672
1	2.773353	–0.282770	–2.250435
1	4.217825	–1.257425	–2.064775

3–BTSH1

SCF energy = –1787.67456147

5	2.321285	–0.762172	–0.554295
8	0.880189	–1.286267	–0.913745
5	–2.476505	–0.969831	–0.529081
15	–0.177042	1.148710	–0.038905
6	–0.617639	2.074035	1.455054
6	–1.886091	2.627972	1.623371

1	–2.633188	2.526651	0.842942
6	–2.192006	3.314986	2.791402
1	–3.178238	3.748202	2.918074
6	–1.236722	3.449470	3.791113
1	–1.477990	3.984964	4.703195
6	0.030483	2.901831	3.622434
1	0.779509	3.009365	4.399225
6	0.344595	2.217621	2.457316
1	1.338673	1.803809	2.321453
6	1.396915	1.777012	–0.661667
6	2.387834	0.829886	–1.009909
6	3.501463	1.372714	–1.668440
1	4.274207	0.702226	–2.021810
6	3.666273	2.733800	–1.885931
1	4.556062	3.092726	–2.394530
6	2.713134	3.641456	–1.437020
1	2.855953	4.708727	–1.568374
6	1.567301	3.154893	–0.832581
1	0.810926	3.848526	–0.474264
6	–1.490667	1.373774	–1.279864
6	–2.403931	0.312592	–1.446812
6	–3.354833	0.439375	–2.467782
1	–4.057105	–0.369158	–2.646435
6	–3.426091	1.576260	–3.262437
1	–4.182769	1.647174	–4.036937
6	–2.513018	2.606883	–3.084311
1	–2.546590	3.486387	–3.718184
6	–1.535886	2.495823	–2.105134
1	–0.795158	3.280261	–2.002578
6	2.429538	–0.942416	1.063111
1	1.705310	–0.307969	1.601995
6	2.067088	–2.396588	1.433216
1	2.223341	–2.567194	2.508201
1	0.993654	–2.517048	1.262985
6	2.792088	–3.503791	0.644759
1	2.232438	–4.439755	0.762298
1	3.767650	–3.699843	1.095693
6	2.977281	–3.218141	–0.855033
1	2.027920	–3.404620	–1.367597
1	3.693967	–3.944497	–1.263241
6	3.435103	–1.779344	–1.170893
1	3.504741	–1.698950	–2.268476
6	4.856873	–1.511454	–0.617841
1	5.522693	–2.337207	–0.905707
1	5.277094	–0.628483	–1.107609
6	4.974358	–1.299571	0.904181
1	5.051036	–2.264786	1.409031
1	5.922279	–0.790995	1.116323
6	3.824034	–0.501047	1.531960
1	3.951843	0.562314	1.286529
1	3.906397	–0.572353	2.625682
6	–2.746273	–0.912686	1.015678
1	–2.618825	0.081205	1.455195
6	–4.271509	–1.227979	1.089806
1	–4.589999	–1.189082	2.138159
1	–4.815800	–0.418890	0.582644
6	–4.685696	–2.571768	0.473877
1	–4.416042	–3.380740	1.153278
1	–5.778051	–2.605773	0.399671
6	–4.086138	–2.830714	–0.918390
1	–4.675980	–2.274939	–1.658442
1	–4.207811	–3.888956	–1.179113
6	–2.588496	–2.435373	–1.082763
1	–2.351897	–2.509676	–2.150937
6	–1.617480	–3.361866	–0.311864
1	–1.760485	–4.395910	–0.649332
1	–0.595176	–3.084131	–0.584819
6	–1.742043	–3.311089	1.218007
1	–2.592895	–3.912995	1.543048
1	–0.863728	–3.798473	1.653528
6	–1.850580	–1.892730	1.800095
1	–0.846836	–1.453661	1.845090
1	–2.192447	–1.951714	2.840881
1	0.141261	–0.360218	–0.199017
1	0.714710	–1.217984	–1.857558

3–BTSH2

SCF energy = –1787.67141792

5	–2.485295	–0.277850	–0.506444
8	–0.882422	–0.311828	–0.765334
5	2.076271	–1.093849	0.277851
15	0.159910	0.951103	–0.003384
6	1.382111	2.278818	–0.418048
6	1.299369	2.888094	–1.670111
1	0.468934	2.660709	–2.332852
6	2.267857	3.797967	–2.070415
1	2.197295	4.266472	–3.046230
6	3.320145	4.113642	–1.217737
1	4.074795	4.828446	–1.528057
6	3.399900	3.516981	0.033987
1	4.213703	3.767841	0.706264
6	2.437941	2.595267	0.433289
1	2.509434	2.127831	1.409742

6	–1.370340	1.957969	0.001008
6	–2.587865	1.299404	–0.227139
6	–3.753077	2.065592	–0.115266
1	–4.719030	1.604250	–0.288311
6	–3.707030	3.411743	0.219646
1	–4.630103	3.978256	0.298092
6	–2.488014	4.040424	0.455136
1	–2.451921	5.092649	0.716835
6	–1.313841	3.313696	0.338968
1	–0.362694	3.806064	0.509361
6	0.476939	0.338609	1.657966
6	1.421924	–0.696462	1.671451
6	1.717902	–1.270174	2.910930
1	2.442204	–2.076012	2.979516
6	1.082756	–0.830735	4.067068
1	1.316827	–1.299802	5.017575
6	0.142488	0.194808	4.020565
1	–0.351978	0.523430	4.928028
6	–0.168545	0.787143	2.805096
1	–0.913947	1.573484	2.744194
6	–3.171973	–0.962728	–1.794773
1	–2.973972	–0.388494	–2.710430
6	–2.557736	–2.365564	–1.999789
1	–3.054261	–2.878485	–2.834149
1	–1.516964	–2.243122	–2.334940
6	–2.589021	–3.294274	–0.769818
1	–1.892810	–4.125446	–0.934642
1	–3.574346	–3.759556	–0.702909
6	–2.260048	–2.624341	0.579202
1	–1.169718	–2.571085	0.708480
1	–2.595486	–3.287264	1.387778
6	–2.832580	–1.208639	0.775160
1	–2.389545	–0.809942	1.698283
6	–4.361976	–1.187535	0.966874
1	–4.646080	–1.833906	1.808322
1	–4.651124	–0.173023	1.266764
6	–5.182749	–1.599798	–0.267702
1	–5.192326	–2.689474	–0.346209
1	–6.230387	–1.318736	–0.108359
6	–4.700643	–0.997522	–1.600455
1	–5.076303	0.028679	–1.686475
1	–5.174433	–1.546331	–2.425913
6	3.557086	–0.657378	–0.087754
1	3.852941	0.273915	0.406347
6	4.450020	–1.779259	0.507484
1	5.500292	–1.581130	0.260362
1	4.387558	–1.713837	1.601250
6	4.086939	–3.209070	0.072694
1	4.493944	–3.405810	–0.920198
1	4.591664	–3.919705	0.736321
6	2.580183	–3.511694	0.081501
1	2.252131	–3.672481	1.116222
1	2.397037	–4.460373	–0.437324
6	1.680617	–2.406394	–0.535190
1	0.649713	–2.747588	–0.363630
6	1.868900	–2.206662	–2.052671
1	1.709975	–3.156986	–2.577090
1	1.073999	–1.537991	–2.410716
6	3.220472	–1.612030	–2.481186
1	3.975685	–2.399645	–2.506626
1	3.135693	–1.263690	–3.516112
6	3.715240	–0.450508	–1.605032
1	3.165029	0.460705	–1.873181
1	4.765324	–0.243790	–1.847543
1	1.191893	0.003496	–0.568535
1	–0.472902	–1.182288	–0.792536

3–BTSH3

SCF energy = –1787.67664308

5	–2.478810	–0.789868	–0.401164
8	–0.783747	–0.085079	–0.826362
5	2.172925	–0.734448	0.182593
15	–0.488205	1.203930	0.098990
6	0.458954	2.396125	–0.836162
6	1.481386	3.111032	–0.214917
1	1.735607	2.911797	0.820353
6	2.194678	4.053716	–0.943378
1	2.999758	4.602660	–0.468558
6	1.895130	4.267796	–2.282071
1	2.465311	4.992891	–2.852781
6	0.874530	3.550949	–2.901273
1	0.651154	3.716614	–3.949071
6	0.148031	2.617563	–2.179973
1	–0.644589	2.051237	–2.657847
6	–2.186797	1.688011	0.308085
6	–3.076660	0.639912	0.018687
6	–4.435530	0.938239	0.170763
1	–5.179301	0.175613	–0.030936
6	–4.860333	2.196576	0.577173
1	–5.922538	2.390961	0.686270
6	–3.946840	3.216266	0.835931
1	–4.291837	4.199180	1.136637
6	–2.592847	2.963812	0.695192

1	–1.862832	3.747948	0.874293
6	0.355030	0.727752	1.590892
6	1.510607	–0.092886	1.535916
6	2.092458	–0.323888	2.794684
1	2.980339	–0.938840	2.848074
6	1.589306	0.192448	3.979536
1	2.094959	–0.028963	4.914631
6	0.439850	0.975463	3.985970
1	0.031267	1.363500	4.912247
6	–0.182562	1.239709	2.781629
1	–1.095034	1.827682	2.766913
6	–2.896705	–1.551438	–1.733487
1	–3.055780	–0.864262	–2.574662
6	–1.777736	–2.535555	–2.137021
1	–2.097029	–3.123734	–3.006850
1	–0.917048	–1.952394	–2.486899
6	–1.315727	–3.502726	–1.031542
1	–0.357490	–3.943233	–1.327074
1	–2.011985	–4.342274	–0.978508
6	–1.155488	–2.876950	0.366656
1	–0.176785	–2.390445	0.429795
1	–1.116621	–3.682296	1.111041
6	–2.226161	–1.844388	0.768639
1	–1.892106	–1.369856	1.700732
6	–3.618750	–2.458846	1.050152
1	–3.537113	–3.207739	1.847423
1	–4.270496	–1.671227	1.450799
6	–4.298699	–3.100734	–0.170184
1	–3.849165	–4.076683	–0.359919
1	–5.346318	–3.309367	0.074781
6	–4.249469	–2.250420	–1.452793
1	–5.029514	–1.481389	–1.399389
1	–4.523364	–2.879225	–2.309460
6	3.404868	0.126173	–0.451995
1	3.170297	1.195995	–0.523737
6	4.642232	0.012397	0.454097
1	5.474871	0.600946	0.042958
1	4.402925	0.477830	1.419816
6	5.138432	–1.422566	0.692028
1	5.710067	–1.743428	–0.182043
1	5.861442	–1.420223	1.516757
6	4.037237	–2.459759	0.993086
1	3.832124	–2.458994	2.068895
1	4.444503	–3.461195	0.794250
6	2.704791	–2.282472	0.231444
1	1.977638	–2.951882	0.712879
6	2.832868	–2.743236	–1.234413
1	3.176415	–3.786373	–1.283723
1	1.832481	–2.733995	–1.686904
6	3.777671	–1.880504	–2.088973
1	4.809507	–2.176167	–1.883321
1	3.620883	–2.119299	–3.147810
6	3.632844	–0.357910	–1.898341
1	2.773288	–0.015246	–2.489861
1	4.513860	0.133084	–2.337108
1	1.311891	–0.769147	–0.738508
1	0.085237	–0.624768	–0.879910

3–BTSH4

SCF energy = –1787.68090604

5	–2.311585	0.833066	–0.183669
8	–0.558667	0.348693	0.045499
5	2.177692	0.858078	–0.683512
15	–0.289726	–1.219514	–0.137583
6	0.222996	–1.988878	1.398257
6	1.431857	–2.677350	1.482210
1	2.082516	–2.743203	0.617270
6	1.809410	–3.249424	2.689292
1	2.754021	–3.776000	2.762817
6	0.986243	–3.129214	3.801923
1	1.287990	–3.570554	4.745793
6	–0.222612	–2.444549	3.715085
1	–0.861670	–2.353267	4.586119
6	–0.611241	–1.876594	2.512688
1	–1.553525	–1.342981	2.439349
6	–1.953117	–1.721191	–0.520541
6	–2.840352	–0.635884	–0.573047
6	–4.174909	–0.960706	–0.860416
1	–4.920448	–0.176524	–0.914817
6	–4.577851	–2.271347	–1.066627
1	–5.619613	–2.479617	–1.288809
6	–3.671798	–3.326049	–0.967670
1	–4.001699	–4.349854	–1.103573
6	–2.347768	–3.051202	–0.681196
1	–1.634640	–3.861986	–0.566381
6	0.930882	–1.445749	–1.420039
6	1.975298	–0.503809	–1.582372
6	2.825953	–0.778702	–2.664249
1	3.617501	–0.076014	–2.890015
6	2.694286	–1.895053	–3.477053
1	3.395544	–2.049433	–4.291529
6	1.664428	–2.804836	–3.270125
1	1.547693	–3.672900	–3.909213

6	0.766495	–2.565141	–2.246818
1	–0.070588	–3.241236	–2.108978
6	–2.767701	1.408616	1.237983
1	–2.774304	0.634595	2.018948
6	–1.801843	2.515102	1.695203
1	–2.151632	2.953586	2.638889
1	–0.840988	2.043386	1.925230
6	–1.580119	3.646357	0.678159
1	–0.690050	4.213895	0.972855
1	–2.406507	4.357408	0.746967
6	–1.407815	3.192744	–0.784153
1	–0.362419	2.912164	–0.941429
1	–1.568803	4.057743	–1.440525
6	–2.304171	2.023927	–1.247447
1	–1.944430	1.700977	–2.233263
6	–3.782043	2.448084	–1.419428
1	–3.839778	3.297648	–2.111297
1	–4.324096	1.635189	–1.916158
6	–4.499169	2.826299	–0.110884
1	–4.222485	3.845951	0.163170
1	–5.579094	2.864195	–0.294764
6	–4.231077	1.886294	1.080816
1	–4.871122	1.000931	0.990406
1	–4.556278	2.384549	2.002936
6	2.438032	0.676218	0.919503
1	1.722331	0.016409	1.422111
6	3.817291	0.029855	1.127247
1	4.002403	–0.152554	2.195055
1	3.803187	–0.960561	0.649654
6	4.989166	0.832494	0.549489
1	5.219969	1.663208	1.219432
1	5.889595	0.206384	0.552129
6	4.751381	1.352739	–0.879306
1	4.975815	0.529469	–1.566618
1	5.499977	2.126092	–1.101283
6	3.333078	1.891941	–1.183172
1	3.281505	2.062366	–2.268677
6	3.076238	3.258167	–0.521049
1	3.829493	3.990764	–0.842690
1	2.112465	3.637057	–0.885172
6	3.049406	3.223894	1.013960
1	4.073693	3.214079	1.393621
1	2.616190	4.159596	1.386935
6	2.261363	2.045714	1.609624
1	1.194244	2.295206	1.558594
1	2.496137	1.966426	2.680482
1	1.106000	1.535061	–0.859913
1	0.269284	0.953192	–0.313079

3–BTSH5

SCF energy = –1786.52606797

5	–2.680416	0.301705	0.420753
8	0.078249	0.126461	0.865720
5	1.828385	1.235339	–0.304680
15	0.088576	–1.112636	–0.007938
6	1.329238	–2.335148	0.496253
6	1.489142	–2.580627	1.859665
1	0.883491	–2.039051	2.579011
6	2.435341	–3.498432	2.292564
1	2.566905	–3.678982	3.353873
6	3.218991	–4.178140	1.366204
1	3.960999	–4.893037	1.705929
6	3.057781	–3.939880	0.006604
1	3.674128	–4.465545	–0.714800
6	2.116126	–3.016361	–0.430273
1	2.009384	–2.810522	–1.490620
6	–1.483281	–2.001396	–0.000233
6	–2.650134	–1.262102	0.248406
6	–3.859434	–1.967499	0.277399
1	–4.785651	–1.438538	0.480172
6	–3.909802	–3.335824	0.045289
1	–4.865336	–3.850121	0.067392
6	–2.742767	–4.048903	–0.198645
1	–2.777250	–5.120172	–0.364786
6	–1.527045	–3.381487	–0.206155
1	–0.608436	–3.939203	–0.358621
6	0.481284	–0.544708	–1.667449
6	1.254528	0.629869	–1.662077
6	1.530181	1.199144	–2.908845
1	2.113127	2.112380	–2.967975
6	1.064185	0.626297	–4.087759
1	1.291626	1.098077	–5.038565
6	0.294554	–0.530666	–4.059489
1	–0.083130	–0.962176	–4.980176
6	–0.006371	–1.116626	–2.837117
1	–0.637379	–1.999882	–2.792328
6	–3.168931	1.038844	1.718447
1	–3.162455	0.391301	2.602668
6	–2.239067	2.236670	1.994091
1	–2.603673	2.796556	2.864959
1	–1.264875	1.826260	2.272487
6	–2.057003	3.203967	0.814696
1	–1.194202	3.846546	1.024288

1	–2.912021	3.882579	0.764877
6	–1.836750	2.528105	–0.550149
1	–0.790695	2.232181	–0.623160
1	–2.003583	3.263118	–1.348844
6	–2.653801	1.254852	–0.826576
1	–2.246243	0.778540	–1.725739
6	–4.167956	1.503285	–1.083714
1	–4.280911	2.142068	–1.967781
1	–4.643785	0.547834	–1.344859
6	–4.914623	2.130911	0.101457
1	–4.657775	3.188756	0.171632
1	–5.991076	2.106289	–0.101828
6	–4.649314	1.435346	1.448140
1	–5.262009	0.526255	1.498893
1	–5.005033	2.074275	2.265917
6	3.089100	0.566890	0.384450
1	3.181100	–0.504085	0.179109
6	4.287869	1.243537	–0.334013
1	5.225023	0.820027	0.047809
1	4.249092	0.971328	–1.397734
6	4.332680	2.772343	–0.209758
1	4.700776	3.042872	0.781118
1	5.076484	3.165496	–0.912075
6	2.984021	3.462540	–0.475671
1	2.847303	3.558004	–1.559515
1	3.023532	4.492069	–0.097659
6	1.727903	2.758863	0.113356
1	0.863777	3.274104	–0.315953
6	1.628616	2.868776	1.646750
1	1.594539	3.926039	1.941725
1	0.673537	2.430718	1.946370
6	2.753327	2.165815	2.418397
1	3.653726	2.784083	2.400498
1	2.469793	2.104501	3.475081
6	3.072291	0.749038	1.913606
1	2.308958	0.069897	2.304296
1	4.028446	0.418019	2.340751

H2O

SCF energy = –76.4094971659

8	0.000000	0.114780	0.000000
1	0.766496	–0.458825	0.000000
1	–0.766496	–0.459417	0.000000

3–BMe1

SCF energy = –1826.99784831

5	–2.675997	–0.207216	–0.534015
8	–1.702478	–0.398803	–1.932966
5	2.214296	–1.321732	0.358174
15	0.346823	0.965582	–0.070808
6	1.646342	2.212849	–0.410411
6	2.581982	2.625488	0.536910
1	2.542961	2.224418	1.543954
6	3.571454	3.541286	0.195488
1	4.296192	3.850960	0.941217
6	3.632750	4.058800	–1.091541
1	4.404964	4.773416	–1.356102
6	2.701817	3.654484	–2.042855
1	2.746113	4.052820	–3.051143
6	1.722272	2.732451	–1.705151
1	1.005837	2.411577	–2.457087
6	–1.189258	1.963603	0.105836
6	–2.447991	1.367125	–0.150252
6	–3.549264	2.231252	–0.092912
1	–4.533643	1.844231	–0.327137
6	–3.444285	3.578094	0.232757
1	–4.335616	4.197597	0.262117
6	–2.201858	4.127762	0.506740
1	–2.100445	5.177882	0.760923
6	–1.077731	3.318591	0.429481
1	–0.100307	3.752941	0.611973
6	0.748620	0.380413	1.614244
6	1.657706	–0.688031	1.683988
6	2.012805	–1.166744	2.947640
1	2.717237	–1.989203	3.038262
6	1.464588	–0.618223	4.101752
1	1.745400	–1.014631	5.072418
6	0.546897	0.420655	4.014507
1	0.105767	0.838726	4.913138
6	0.190256	0.921960	2.768781
1	–0.533572	1.726842	2.693761
6	–4.166916	–0.678571	–0.939466
1	–4.671846	0.031113	–1.613233
6	–4.111726	–2.029387	–1.679915
1	–5.128519	–2.360171	–1.930715
1	–3.600188	–1.888859	–2.639773
6	–3.403111	–3.151534	–0.907115
1	–3.186739	–3.976686	–1.595431
1	–4.091423	–3.568554	–0.169311
6	–2.095084	–2.723757	–0.220520
1	–1.303822	–2.722662	–0.978058
1	–1.806800	–3.495279	0.506711

6	–2.097138	–1.338035	0.461868
1	–1.063209	–1.158771	0.774389
6	–2.937838	–1.271907	1.750304
1	–2.558653	–1.992053	2.486832
1	–2.795038	–0.279950	2.199095
6	–4.436360	–1.517551	1.534223
1	–4.611112	–2.588684	1.416743
1	–4.981470	–1.235964	2.442471
6	–5.038559	–0.751102	0.342264
1	–5.254080	0.266862	0.680996
1	–6.014103	–1.190837	0.095208
6	3.544348	–0.856557	–0.334463
1	3.890905	0.123762	0.008266
6	4.565315	–1.909046	0.195527
1	5.549516	–1.707231	–0.244066
1	4.685694	–1.751194	1.275645
6	4.182408	–3.377238	–0.054099
1	4.406012	–3.643917	–1.087821
1	4.828032	–4.018388	0.555940
6	2.713923	–3.709210	0.262533
1	2.596309	–3.805309	1.349622
1	2.463475	–4.694563	–0.148406
6	1.672150	–2.666116	–0.243431
1	0.702345	–2.957408	0.170992
6	1.544272	–2.593102	–1.777031
1	1.289439	–3.582350	–2.177747
1	0.682964	–1.953768	–2.006286
6	2.773708	–2.046071	–2.518202
1	3.522051	–2.834593	–2.618349
1	2.484933	–1.797175	–3.545531
6	3.407537	–0.806890	–1.868084
1	2.798685	0.072441	–2.111003
1	4.388671	–0.622877	–2.324000
1	–0.789526	–0.259813	–1.600333
6	–1.949918	0.453671	–3.052621
1	–1.286136	0.162417	–3.867100
1	–2.985237	0.296428	–3.345210
1	–1.800744	1.501425	–2.782409

3–BMe2

SCF energy = –1826.98396372

5	–2.660733	–0.326676	–0.699047
8	–1.630160	–0.406984	–1.821491
5	2.577141	–0.971935	0.483794
15	0.078329	0.957559	0.236971
6	1.381866	2.022474	–0.424294
6	2.357336	2.593343	0.391709
1	2.364502	2.392919	1.457828
6	3.335795	3.405758	–0.167640
1	4.096885	3.845706	0.467178
6	3.344685	3.643149	–1.536495
1	4.115184	4.270692	–1.971250
6	2.371302	3.074852	–2.352163
1	2.380095	3.257722	–3.420846
6	1.388602	2.267043	–1.799641
1	0.626676	1.826191	–2.435584
6	–1.460578	1.860058	0.357781
6	–2.630924	1.242454	–0.130184
6	–3.753402	2.084834	–0.143467
1	–4.678964	1.708133	–0.561914
6	–3.732480	3.387704	0.334646
1	–4.638326	3.985945	0.299407
6	–2.561628	3.940410	0.845866
1	–2.542369	4.958646	1.219107
6	–1.410194	3.175387	0.835703
1	–0.472600	3.604586	1.180254
6	0.681636	0.293463	1.800484
6	1.859167	–0.477482	1.791534
6	2.353523	–0.895084	3.029824
1	3.272469	–1.472749	3.070479
6	1.684394	–0.603874	4.214478
1	2.082397	–0.960822	5.158688
6	0.515764	0.143821	4.192937
1	–0.008822	0.368853	5.114750
6	0.018680	0.609787	2.981611
1	–0.891727	1.199324	2.954090
6	–4.137120	–0.846728	–1.181881
1	–4.598097	–0.164277	–1.914884
6	–3.947939	–2.193803	–1.906013
1	–4.913655	–2.577359	–2.266341
1	–3.336174	–2.021954	–2.798340
6	–3.272434	–3.284992	–1.060409
1	–2.952485	–4.100018	–1.721230
1	–4.009425	–3.735022	–0.390866
6	–2.057020	–2.801920	–0.250625
1	–1.208203	–2.732865	–0.939951
1	–1.793445	–3.571360	0.490435
6	–2.204380	–1.425555	0.430333
1	–1.216410	–1.224725	0.874792
6	–3.181874	–1.401611	1.615594
1	–2.863227	–2.108733	2.394986
1	–3.133198	–0.404059	2.075969
6	–4.639540	–1.700108	1.244465

1	–4.762119	–2.776822	1.110141
1	–5.287048	–1.441715	2.091470
6	–5.136100	–0.953073	–0.006019
1	–5.424705	0.054775	0.310431
1	–6.067487	–1.426377	–0.349331
6	4.113683	–0.824926	0.201214
1	4.616187	–0.153567	0.907660
6	4.733639	–2.239613	0.380754
1	5.782176	–2.219529	0.059121
1	4.758181	–2.464277	1.454944
6	3.989737	–3.378144	–0.336478
1	4.276860	–3.413239	–1.388346
1	4.316893	–4.334026	0.086143
6	2.463204	–3.282683	–0.225913
1	2.157354	–3.543423	0.796510
1	1.994512	–4.031677	–0.873716
6	1.867768	–1.883720	–0.576022
1	0.786941	–1.975523	–0.437431
6	2.135165	–1.428965	–2.025435
1	1.821945	–2.216570	–2.720641
1	1.468590	–0.584824	–2.234691
6	3.581832	–1.009492	–2.341711
1	4.173917	–1.887445	–2.607132
1	3.576909	–0.386087	–3.242519
6	4.289878	–0.236669	–1.219184
1	3.916776	0.793382	–1.207904
1	5.359345	–0.162623	–1.452145
1	–0.163766	–0.025097	–0.745154
6	–1.842972	0.369545	–2.955499
1	–1.034360	0.184882	–3.673870
1	–2.791163	0.125989	–3.454722
1	–1.867145	1.450728	–2.731108

3–BMe3

SCF energy = –1826.96479839

5	–2.935851	–0.443010	–0.410877
8	–0.679504	0.182172	–1.233105
5	2.361895	–0.735086	0.135775
15	–0.168914	1.014718	0.049609
6	0.897549	2.377878	–0.439844
6	1.975601	2.750862	0.358158
1	2.200011	2.193323	1.259644
6	2.771667	3.820538	–0.025025
1	3.618508	4.105238	0.589217
6	2.495926	4.509558	–1.200461
1	3.128942	5.336859	–1.503032
6	1.412513	4.141740	–1.990857
1	1.196072	4.681760	–2.906037
6	0.604495	3.080365	–1.608625
1	–0.251392	2.801822	–2.215673
6	–1.777749	1.773152	0.411748
6	–2.947580	1.040265	0.139875
6	–4.164705	1.665400	0.432158
1	–5.096231	1.147285	0.229960
6	–4.221171	2.939221	0.985164
1	–5.184403	3.388416	1.204403
6	–3.052509	3.642668	1.241789
1	–3.091250	4.641431	1.662519
6	–1.828901	3.060080	0.943643
1	–0.912228	3.612421	1.125139
6	0.328885	0.120719	1.524045
6	1.474172	–0.698378	1.485962
6	1.760275	–1.372242	2.686967
1	2.621793	–2.026348	2.732940
6	0.982845	–1.235399	3.824746
1	1.248038	–1.781978	4.725145
6	–0.133580	–0.401478	3.828562
1	–0.739786	–0.289170	4.720740
6	–0.466026	0.277349	2.673487
1	–1.344790	0.910720	2.664632
6	–3.721785	–0.911438	–1.695500
1	–3.956124	–0.087652	–2.380034
6	–2.928730	–1.977924	–2.481246
1	–3.571001	–2.403666	–3.262723
1	–2.123147	–1.469815	–3.016198
6	–2.326879	–3.127479	–1.651831
1	–1.539908	–3.608937	–2.242772
1	–3.082465	–3.902049	–1.506745
6	–1.740672	–2.722874	–0.288492
1	–0.730997	–2.322117	–0.427364
1	–1.612507	–3.623414	0.324242
6	–2.543811	–1.669249	0.496252
1	–1.958447	–1.396542	1.377533
6	–3.920209	–2.166381	1.027523
1	–3.758196	–3.034604	1.676912
1	–4.337966	–1.383956	1.676057
6	–4.951238	–2.517884	–0.053726
1	–4.705656	–3.483984	–0.496677
1	–5.929788	–2.655677	0.419033
6	–5.077075	–1.458210	–1.158011
1	–5.673677	–0.620190	–0.778504
1	–5.651787	–1.868405	–1.997279
6	3.877855	–0.145675	0.297756

1	3.894090	0.816542	0.829816
6	4.757807	–1.101610	1.128936
1	5.805152	–0.766093	1.110089
1	4.450827	–1.009480	2.177045
6	4.723566	–2.591041	0.722651
1	5.459340	–2.762679	–0.066384
1	5.074830	–3.195997	1.567966
6	3.359702	–3.134561	0.252603
1	2.751333	–3.404724	1.123233
1	3.533657	–4.081406	–0.278932
6	2.539972	–2.170754	–0.624291
1	1.570496	–2.663530	–0.802072
6	3.186594	–1.948138	–2.007924
1	3.391308	–2.913737	–2.493080
1	2.459663	–1.444000	–2.654947
6	4.475804	–1.109077	–2.019391
1	5.326128	–1.734053	–1.735979
1	4.684696	–0.794638	–3.049556
6	4.433398	0.126610	–1.110460
1	3.799496	0.894370	–1.577099
1	5.443917	0.557840	–1.056326
1	1.728873	0.040090	–0.613731
6	0.072769	–0.231227	–2.380198
1	0.302455	–1.290240	–2.286593
1	–0.568271	–0.043976	–3.240122
1	0.997267	0.334936	–2.469050

3–BMe4

SCF energy = –1826.95484547

5	–2.866407	0.591752	0.404045
8	–0.536705	–0.179739	1.246564
5	2.162650	1.333394	–0.046432
15	–0.233267	–1.095590	–0.020302
6	0.791817	–2.502297	0.426379
6	1.863699	–2.870838	–0.382956
1	2.119588	–2.270949	–1.248553
6	2.618702	–3.988271	–0.054082
1	3.461470	–4.267704	–0.675792
6	2.303837	–4.731187	1.076765
1	2.901167	–5.598647	1.336540
6	1.225570	–4.369983	1.879663
1	0.980199	–4.954223	2.759513
6	0.462561	–3.260306	1.552824
1	–0.387907	–2.985697	2.169419
6	–1.887121	–1.751471	–0.323097
6	–2.986984	–0.919393	–0.048327
6	–4.256219	–1.471923	–0.254825
1	–5.138716	–0.876785	–0.044653
6	–4.424511	–2.765751	–0.732207
1	–5.425195	–3.155191	–0.888837
6	–3.320756	–3.566396	–0.994610
1	–3.448156	–4.580590	–1.356373
6	–2.048080	–3.060499	–0.775953
1	–1.181255	–3.687750	–0.957712
6	0.352042	–0.190225	–1.442755
6	1.319251	0.846208	–1.373513
6	1.480927	1.534664	–2.591770
1	2.149717	2.384778	–2.610047
6	0.830241	1.202289	–3.767645
1	1.017429	1.782707	–4.666463
6	–0.059963	0.134184	–3.805424
1	–0.570336	–0.141857	–4.721467
6	–0.314269	–0.544946	–2.632881
1	–1.057123	–1.334322	–2.640414
6	–3.536614	1.176982	1.702061
1	–3.778379	0.409334	2.446909
6	–2.606781	2.217702	2.362595
1	–3.126851	2.687140	3.207414
1	–1.757729	1.684228	2.799799
6	–2.072635	3.313868	1.427721
1	–1.235315	3.816098	1.923801
1	–2.834766	4.086268	1.303502
6	–1.590819	2.812861	0.056345
1	–0.581980	2.406359	0.167283
1	–1.493521	3.666972	–0.625156
6	–2.455617	1.722334	–0.603651
1	–1.923175	1.357225	–1.486479
6	–3.850811	2.210437	–1.101760
1	–3.701499	2.998260	–1.848979
1	–4.339151	1.383574	–1.636358
6	–4.790282	2.719321	0.000646
1	–4.473131	3.713631	0.316344
1	–5.792455	2.854059	–0.420841
6	–4.886583	1.788753	1.221889
1	–5.576432	0.969206	0.986048
1	–5.350121	2.326412	2.058056
6	3.098925	0.171666	0.644690
1	2.547482	–0.740123	0.908775
6	4.186808	–0.275799	–0.347751
1	4.781529	–1.105585	0.064698
1	3.693085	–0.672771	–1.246534
6	5.139062	0.843032	–0.786687
1	5.859724	1.031229	0.011993

1	5.739437	0.491951	–1.635288
6	4.429097	2.150957	–1.184232
1	4.099301	2.034579	–2.222962
1	5.175238	2.959016	–1.206823
6	3.217908	2.561618	–0.314140
1	2.732466	3.408061	–0.825329
6	3.654731	3.104679	1.058101
1	4.325168	3.969626	0.943967
1	2.758786	3.475572	1.571656
6	4.351292	2.070447	1.953496
1	5.391626	1.964484	1.637142
1	4.406858	2.458128	2.978528
6	3.670978	0.689962	1.982530
1	2.842276	0.749518	2.698569
1	4.377287	–0.040580	2.406515
1	1.313606	1.729852	0.754669
6	0.204130	–0.030860	2.468060
1	0.540937	1.000136	2.521004
1	–0.479161	–0.278103	3.280267
1	1.068212	–0.692409	2.483623

3–BTSMe1

SCF energy = –1826.98200493

5	–2.654902	–0.313829	–0.662668
8	–1.504495	–0.501862	–1.710677
5	2.538977	–1.007576	0.508589
15	0.090141	0.947668	0.157946
6	1.435336	2.012824	–0.435333
6	2.374978	2.567171	0.434608
1	2.318054	2.363634	1.498455
6	3.396474	3.366580	–0.062684
1	4.126760	3.790103	0.618140
6	3.487245	3.613770	–1.426809
1	4.291044	4.231073	–1.813404
6	2.551647	3.065877	–2.297972
1	2.623597	3.253551	–3.363580
6	1.529804	2.267134	–1.805464
1	0.804564	1.838115	–2.489791
6	–1.427241	1.906706	0.289003
6	–2.602599	1.281308	–0.186619
6	–3.722581	2.123256	–0.236430
1	–4.647087	1.738174	–0.648756
6	–3.699540	3.442562	0.197815
1	–4.602816	4.042452	0.136309
6	–2.530076	4.005314	0.697339
1	–2.508856	5.035865	1.035578
6	–1.380477	3.234733	0.721553
1	–0.442861	3.669539	1.057928
6	0.645816	0.310500	1.759641
6	1.804638	–0.487224	1.794104
6	2.268307	–0.889683	3.049719
1	3.175454	–1.483542	3.118584
6	1.582632	–0.563376	4.215111
1	1.953529	–0.910027	5.174169
6	0.431083	0.208619	4.153227
1	–0.106764	0.464505	5.059532
6	–0.030214	0.663108	2.923276
1	–0.924259	1.275284	2.867744
6	–4.077739	–0.833350	–1.268338
1	–4.465758	–0.169472	–2.057984
6	–3.848192	–2.211374	–1.920308
1	–4.783823	–2.589563	–2.355919
1	–3.149742	–2.094859	–2.756284
6	–3.285974	–3.275415	–0.964681
1	–2.924479	–4.127392	–1.553159
1	–4.098540	–3.677257	–0.355148
6	–2.143925	–2.783118	–0.058106
1	–1.223516	–2.786662	–0.651928
1	–1.989366	–3.516746	0.746474
6	–2.304697	–1.366769	0.535271
1	–1.347972	–1.153598	1.033955
6	–3.374585	–1.260525	1.632677
1	–3.133164	–1.926434	2.473053
1	–3.349292	–0.239894	2.039711
6	–4.797565	–1.568693	1.151245
1	–4.920190	–2.650655	1.069399
1	–5.514332	–1.257515	1.920623
6	–5.177726	–0.892012	–0.178841
1	–5.503246	0.125999	0.054937
1	–6.068758	–1.391983	–0.584355
6	4.087732	–0.919824	0.269591
1	4.596583	–0.277815	0.998343
6	4.647565	–2.359485	0.444362
1	5.704142	–2.378546	0.149650
1	4.634596	–2.597155	1.516004
6	3.878266	–3.460649	–0.304529
1	4.191290	–3.496053	–1.349175
1	4.156141	–4.433075	0.115632
6	2.353814	–3.306430	–0.233462
1	2.009960	–3.565218	0.777240
1	1.874957	–4.030626	–0.902175
6	1.826157	–1.881429	–0.581737
1	0.739049	–1.924145	–0.473167

6	2.151102	–1.420550	–2.016508
1	1.826895	–2.185418	–2.732375
1	1.527525	–0.544391	–2.227290
6	3.619988	–1.050397	–2.288137
1	4.188124	–1.945847	–2.547622
1	3.662530	–0.416504	–3.180732
6	4.321648	–0.316422	–1.135970
1	3.981448	0.725228	–1.118514
1	5.398769	–0.274030	–1.340112
1	–0.414815	–0.034561	–0.911340
6	–1.586957	0.224253	–2.907041
1	–0.743167	–0.051252	–3.548162
1	–2.514428	–0.009745	–3.437798
1	–1.569179	1.311395	–2.733523

3–BTSMe2

SCF energy = –1826.95607279

5	2.603288	–0.554029	0.317827
8	1.098224	–0.193238	1.089185
5	–2.495178	–0.725383	–0.447851
15	0.035091	0.837558	0.009907
6	–0.734645	2.089931	1.092386
6	–1.940842	2.705371	0.767595
1	–2.439351	2.467751	–0.165198
6	–2.495787	3.642701	1.631269
1	–3.432761	4.123272	1.370883
6	–1.852749	3.965422	2.819389
1	–2.289812	4.694793	3.493165
6	–0.640352	3.363896	3.137508
1	–0.126196	3.624944	4.056216
6	–0.078115	2.435015	2.273957
1	0.884199	1.990874	2.506115
6	1.633125	1.672693	–0.377789
6	2.820370	0.953508	–0.210486
6	4.005284	1.624985	–0.530570
1	4.958702	1.119272	–0.442636
6	4.004658	2.948874	–0.952238
1	4.945848	3.440335	–1.179436
6	2.811700	3.653663	–1.062231
1	2.810763	4.695703	–1.364841
6	1.618061	3.009719	–0.773476
1	0.680682	3.554240	–0.847350
6	–0.793335	0.852457	–1.637824
6	–2.012751	0.158672	–1.666745
6	–2.773526	0.232103	–2.841269
1	–3.736268	–0.265280	–2.897936
6	–2.302894	0.899950	–3.963328
1	–2.901616	0.919506	–4.868630
6	–1.057371	1.515790	–3.940088
1	–0.672449	2.010790	–4.825096
6	–0.303906	1.495328	–2.776415
1	0.667551	1.972101	–2.762406
6	3.646811	–1.262386	1.324968
1	3.895908	–0.630116	2.189010
6	3.141997	–2.618132	1.870210
1	3.978263	–3.141930	2.352415
1	2.430165	–2.441650	2.679029
6	2.511916	–3.574246	0.833477
1	1.871783	–4.293655	1.358282
1	3.300302	–4.179993	0.382059
6	1.694184	–2.910362	–0.290883
1	0.685723	–2.688666	0.076570
1	1.548139	–3.647361	–1.092231
6	2.279624	–1.607460	–0.858755
1	1.542125	–1.209526	–1.574562
6	3.592157	–1.791792	–1.649847
1	3.450841	–2.522145	–2.457543
1	3.820780	–0.839022	–2.142754
6	4.805877	–2.218335	–0.805593
1	4.754700	–3.293234	–0.618448
1	5.718029	–2.075402	–1.396239
6	4.962318	–1.477187	0.535346
1	5.440718	–0.511049	0.360613
1	5.670139	–2.035864	1.161870
6	–3.680076	–0.307452	0.513297
1	–3.823699	0.775102	0.582171
6	–4.957957	–0.879204	–0.165672
1	–5.820038	–0.709368	0.491317
1	–5.155166	–0.284625	–1.066175
6	–4.900311	–2.366756	–0.555596
1	–5.105367	–2.985803	0.319461
1	–5.715879	–2.579351	–1.255554
6	–3.571979	–2.805955	–1.190561
1	–3.530308	–2.459746	–2.230101
1	–3.539826	–3.900836	–1.244925
6	–2.304506	–2.298187	–0.447856
1	–1.437627	–2.619277	–1.036615
6	–2.165023	–2.882113	0.970270
1	–2.258516	–3.974796	0.929802
1	–1.141346	–2.692664	1.299898
6	–3.135153	–2.337326	2.035034
1	–4.074572	–2.892400	1.995563
1	–2.721850	–2.551516	3.027150

6	–3.438969	–0.834352	1.938349
1	–2.607399	–0.259650	2.365561
1	–4.305140	–0.605597	2.572156
1	–0.934282	–0.242832	0.356126
6	0.551488	–0.813344	2.238416
1	0.513085	–1.892994	2.120448
1	1.173280	–0.553950	3.096231
1	–0.460918	–0.441724	2.409096

3–BTSMe3

SCF energy = –1826.90369316

5	–2.836036	–0.602531	0.126811
8	–1.100807	–0.593167	–0.028163
5	2.814079	–0.809339	0.755783
15	–0.432419	0.857745	0.017312
6	0.330396	1.191263	–1.571197
6	1.297069	2.188117	–1.681769
1	1.639237	2.719785	–0.799938
6	1.864289	2.454182	–2.919317
1	2.634412	3.212053	–3.006193
6	1.469721	1.725287	–4.034755
1	1.930322	1.920860	–4.997053
6	0.492958	0.740931	–3.923337
1	0.188525	0.174356	–4.796194
6	–0.088283	0.476048	–2.692615
1	–0.843078	–0.297200	–2.594103
6	–1.924904	1.822253	0.141599
6	–3.056714	0.997369	0.186431
6	–4.288946	1.669571	0.217516
1	–5.212391	1.104757	0.256989
6	–4.364250	3.053460	0.188216
1	–5.336544	3.535327	0.212803
6	–3.212060	3.836514	0.112622
1	–3.284036	4.917627	0.071101
6	–1.977959	3.216138	0.081311
1	–1.067486	3.804465	0.013976
6	0.746576	1.073255	1.388159
6	2.006725	0.402746	1.593284
6	2.636329	0.779791	2.792991
1	3.569685	0.299799	3.047806
6	2.148265	1.710431	3.698259
1	2.719218	1.935410	4.594005
6	0.932470	2.328699	3.469841
1	0.519377	3.045707	4.170543
6	0.235891	1.992803	2.324879
1	–0.733292	2.449075	2.170150
6	–3.371340	–1.363372	–1.183566
1	–3.135806	–0.808228	–2.103299
6	–2.693295	–2.740701	–1.290297
1	–3.096121	–3.296195	–2.147259
1	–1.633635	–2.577561	–1.521963
6	–2.815879	–3.625506	–0.035601
1	–2.083695	–4.439552	–0.100560
1	–3.787330	–4.123451	–0.054485
6	–2.643482	–2.906169	1.319019
1	–1.580447	–2.853020	1.570097
1	–3.082192	–3.537839	2.102585
6	–3.228709	–1.481915	1.412330
1	–2.858637	–1.035534	2.345742
6	–4.770843	–1.491388	1.495779
1	–5.091778	–2.111715	2.342523
1	–5.115081	–0.478694	1.733076
6	–5.478066	–1.992687	0.223974
1	–5.447584	–3.084273	0.208097
1	–6.542968	–1.740246	0.285460
6	–4.911755	–1.446247	–1.101125
1	–5.315764	–0.443224	–1.277555
1	–5.295263	–2.059865	–1.926860
6	3.124074	–0.586121	–0.830431
1	2.266174	–0.239170	–1.414704
6	4.179733	0.526961	–0.977852
1	4.369541	0.734228	–2.040687
1	3.754568	1.451028	–0.562664
6	5.514092	0.254906	–0.274154
1	6.101538	–0.448974	–0.866946
1	6.104479	1.179057	–0.258804
6	5.358810	–0.261863	1.164472
1	5.162584	0.606032	1.805372
1	6.322774	–0.666010	1.504210
6	4.240126	–1.307598	1.380311
1	4.177150	–1.492412	2.462444
6	4.585557	–2.676068	0.759447
1	5.540025	–3.046209	1.159568
1	3.822426	–3.392431	1.088004
6	4.656145	–2.699809	–0.774623
1	5.622632	–2.309118	–1.100100
1	4.641343	–3.741305	–1.117460
6	3.526595	–1.928209	–1.474436
1	2.631170	–2.566328	–1.485624
1	3.796432	–1.778803	–2.529575
1	2.061307	–1.880277	0.868276
6	0.336235	–1.676372	0.344757
1	0.310820	–1.398751	1.379358

1	0.008582	–2.674515	0.081452
1	0.917909	–1.170354	–0.399690

CH4

SCF energy = –40.5095531263

6	0.000000	0.000000	0.000086
1	0.000000	1.028015	–0.363661
1	0.890287	–0.514007	–0.363661
1	–0.890287	–0.514007	–0.363661
1	0.000000	0.000000	1.090469

3–BPh1

SCF energy = –2018.71086158

5	–2.502693	–0.774277	0.021876
8	–1.633064	0.072247	–1.395275
5	2.604435	–1.163640	–0.348841
15	0.438853	0.511588	0.790740
6	1.442026	2.023849	1.048021
6	2.597547	2.050804	1.826193
1	2.913269	1.159069	2.356939
6	3.352826	3.215626	1.921096
1	4.252767	3.223097	2.527513
6	2.957516	4.363014	1.247260
1	3.547124	5.270711	1.323518
6	1.799770	4.345700	0.475131
1	1.481114	5.239427	–0.051302
6	1.050823	3.183358	0.371378
1	0.149582	3.178539	–0.234734
6	–1.147858	0.909730	1.635377
6	–2.363750	0.346866	1.181411
6	–3.525598	0.800966	1.818411
1	–4.488260	0.433947	1.481520
6	–3.509304	1.717571	2.861610
1	–4.441599	2.033720	3.319363
6	–2.302008	2.232367	3.306918
1	–2.269655	2.950760	4.119548
6	–1.129049	1.835551	2.681872
1	–0.186878	2.265899	3.005194
6	1.271120	–0.748934	1.816215
6	2.294905	–1.457932	1.165412
6	2.997568	–2.417167	1.899835
1	3.802073	–2.978138	1.431999
6	2.673711	–2.682389	3.225725
1	3.225013	–3.440186	3.773521
6	1.639413	–1.992702	3.845867
1	1.378507	–2.208699	4.876511
6	0.939773	–1.021441	3.140690
1	0.127787	–0.481588	3.617108
6	–3.958448	–1.203013	–0.502127
1	–4.662851	–0.363313	–0.580908
6	–3.857382	–1.833492	–1.902755
1	–4.853850	–2.140752	–2.246721
1	–3.519458	–1.066422	–2.608463
6	–2.913988	–3.041680	–1.982679
1	–2.715431	–3.268599	–3.036218
1	–3.426871	–3.923213	–1.592798
6	–1.569817	–2.852718	–1.257961
1	–0.907621	–2.294620	–1.926982
1	–1.094652	–3.834231	–1.125427
6	–1.612488	–2.110413	0.096798
1	–0.569654	–1.929958	0.381728
6	–2.218172	–2.943946	1.245120
1	–1.623878	–3.852820	1.401301
1	–2.133385	–2.364872	2.173814
6	–3.684152	–3.332411	1.020386
1	–3.730732	–4.158661	0.308808
1	–4.098077	–3.732608	1.952835
6	–4.576681	–2.172510	0.544779
1	–4.864889	–1.593129	1.428115
1	–5.512519	–2.583741	0.143912
6	3.693338	–0.137556	–0.828085
1	4.007235	0.557298	–0.042958
6	4.916203	–1.053259	–1.138464
1	5.733699	–0.438526	–1.534113
1	5.284550	–1.458332	–0.186450
6	4.637599	–2.223410	–2.096868
1	4.621345	–1.864572	–3.126931
1	5.475991	–2.926805	–2.048893
6	3.336616	–2.981655	–1.792435
1	3.492083	–3.620768	–0.913435
1	3.105382	–3.666679	–2.616762
6	2.098733	–2.074095	–1.523611
1	1.276903	–2.734960	–1.231297
6	1.651507	–1.254538	–2.749651
1	1.479394	–1.924683	–3.601317
1	0.668617	–0.828520	–2.520595
6	2.589805	–0.115771	–3.182227
1	3.391582	–0.514957	–3.805894
1	2.035703	0.562813	–3.841495
6	3.193467	0.694035	–2.024714
1	2.442077	1.395789	–1.640977
1	4.008823	1.319086	–2.409825

1	–0.706273	0.002132	–1.072340
6	–1.828302	1.349041	–1.887237
6	–0.771584	1.994236	–2.518552
6	–3.064816	1.960534	–1.756601
6	–0.959465	3.273668	–3.024826
6	–3.240667	3.237394	–2.274457
6	–2.194090	3.899805	–2.905250
1	0.189584	1.499135	–2.611456
1	–3.869892	1.447727	–1.248583
1	–0.133021	3.777125	–3.514952
1	–4.206589	3.720143	–2.173093
1	–2.341057	4.897222	–3.304441

3–BPh2

SCF energy = –2018.71357960

5	–2.650498	–0.347856	–0.443579
8	–1.720973	0.609444	–1.222453
5	2.914243	–1.014847	–0.394338
15	0.218464	–0.079167	1.010806
6	1.368639	1.230373	1.486089
6	2.384311	1.006379	2.415946
1	2.529277	0.019622	2.842892
6	3.224106	2.050103	2.782358
1	4.015579	1.876288	3.502874
6	3.054760	3.309211	2.218656
1	3.718578	4.119602	2.500331
6	2.040816	3.532406	1.292742
1	1.904362	4.512556	0.850299
6	1.190952	2.499090	0.927453
1	0.396748	2.685080	0.210394
6	–1.336895	0.113960	1.874067
6	–2.553060	0.015725	1.169449
6	–3.689438	0.270161	1.953389
1	–4.659539	0.270649	1.472078
6	–3.631415	0.553482	3.309835
1	–4.550391	0.738713	3.857899
6	–2.407825	0.620357	3.969305
1	–2.355617	0.849838	5.027921
6	–1.252289	0.416930	3.239688
1	–0.285320	0.509999	3.727317
6	1.023323	–1.661294	1.329086
6	2.258890	–1.925687	0.707817
6	2.891608	–3.126292	1.041293
1	3.856067	–3.361152	0.601285
6	2.306576	–4.040230	1.911703
1	2.814032	–4.973279	2.133432
6	1.081588	–3.760755	2.499689
1	0.622057	–4.471327	3.177419
6	0.442956	–2.558650	2.220447
1	–0.512390	–2.329626	2.680381
6	–4.142900	–0.343239	–1.106159
1	–4.679660	0.598967	–0.911452
6	–3.966188	–0.431461	–2.636355
1	–4.946917	–0.434031	–3.132464
1	–3.457964	0.476086	–2.977010
6	–3.173513	–1.659073	–3.121603
1	–2.869565	–1.494318	–4.162328
1	–3.840287	–2.524199	–3.156606
6	–1.922035	–2.005795	–2.292090
1	–1.107854	–1.349007	–2.617378
1	–1.607179	–3.030414	–2.538911
6	–2.060204	–1.840479	–0.765127
1	–1.047244	–2.001701	–0.359559
6	–2.940022	–2.904299	–0.089725
1	–2.528686	–3.909359	–0.259548
1	–2.900494	–2.742665	0.997354
6	–4.406786	–2.886770	–0.536841
1	–4.486429	–3.354440	–1.520299
1	–4.995618	–3.526007	0.132213
6	–5.037725	–1.483743	–0.566416
1	–5.352531	–1.247145	0.455107
1	–5.968807	–1.530072	–1.148855
6	4.407914	–0.531604	–0.373927
1	4.892273	–0.681646	0.598213
6	5.159207	–1.417967	–1.409692
1	6.179119	–1.035473	–1.538010
1	5.272330	–2.422003	–0.981446
6	4.477460	–1.546905	–2.782336
1	4.711799	–0.679188	–3.399834
1	4.908719	–2.403889	–3.310267
6	2.955942	–1.727059	–2.706547
1	2.729400	–2.746080	–2.365123
1	2.521591	–1.648586	–3.709310
6	2.219193	–0.720241	–1.768897
1	1.160128	–0.996844	–1.809385
6	2.352844	0.756707	–2.189109
1	2.039225	0.874414	–3.233544
1	1.630977	1.334882	–1.603089
6	3.740939	1.388026	–1.998627
1	4.379127	1.158537	–2.853978
1	3.629598	2.477549	–2.006643
6	4.451804	0.979649	–0.701108
1	3.998342	1.521458	0.135676

1	5.496206	1.312925	–0.741960
1	–0.034205	0.082238	–0.354483
6	–1.729649	1.937177	–1.250997
6	–0.852096	2.556047	–2.158572
6	–2.495745	2.757999	–0.410260
6	–0.704237	3.933419	–2.186373
6	–2.339194	4.139076	–0.449380
6	–1.438819	4.740452	–1.320712
1	–0.291862	1.918666	–2.834006
1	–3.201961	2.315490	0.278820
1	–0.013274	4.380786	–2.895047
1	–2.936846	4.753335	0.217600
1	–1.325549	5.819118	–1.340805

3–BPh3

SCF energy = –2018.67394294

5	2.740201	–0.885262	0.233274
8	0.469818	0.406459	0.737429
5	–2.452266	–0.820623	–0.121484
15	0.228564	0.777824	–0.827357
6	–0.726693	2.289091	–1.033098
6	–1.973388	2.226509	–1.655777
1	–2.365843	1.274937	–1.991445
6	–2.722758	3.382902	–1.811117
1	–3.695709	3.327609	–2.285697
6	–2.235642	4.597417	–1.342827
1	–2.829243	5.498471	–1.456099
6	–0.990799	4.663167	–0.727053
1	–0.610738	5.608946	–0.357404
6	–0.230405	3.513477	–0.575860
1	0.737991	3.572576	–0.092454
6	1.934077	1.121018	–1.331007
6	2.953941	0.335006	–0.755208
6	4.266022	0.617521	–1.151337
1	5.087243	0.050077	–0.724399
6	4.553541	1.604856	–2.086814
1	5.584049	1.789608	–2.372319
6	3.531737	2.358142	–2.647191
1	3.751827	3.132328	–3.373670
6	2.220153	2.119334	–2.260918
1	1.418573	2.713630	–2.686548
6	–0.369978	–0.621443	–1.758565
6	–1.537159	–1.317173	–1.371078
6	–1.846797	–2.418801	–2.193112
1	–2.712674	–3.020894	–1.952772
6	–1.104619	–2.768401	–3.307815
1	–1.402866	–3.627490	–3.901837
6	0.013790	–2.025877	–3.680154
1	0.592013	–2.289047	–4.558972
6	0.387851	–0.954572	–2.896993
1	1.277724	–0.394919	–3.160431
6	3.339075	–0.974951	1.688605
1	3.673142	–0.012373	2.090789
6	2.273878	–1.544949	2.654099
1	2.728415	–1.696061	3.641207
1	1.502315	–0.782643	2.797182
6	1.601665	–2.851474	2.202557
1	0.688965	–2.993017	2.790566
1	2.241956	–3.698457	2.458427
6	1.226678	–2.904479	0.713169
1	0.284616	–2.369828	0.569531
1	1.022090	–3.944092	0.429057
6	2.248059	–2.292377	–0.265392
1	1.786875	–2.271406	–1.254427
6	3.571381	–3.099228	–0.415098
1	3.331398	–4.102483	–0.785817
1	4.177095	–2.629179	–1.203053
6	4.410847	–3.207457	0.863019
1	3.951722	–3.927017	1.541694
1	5.391694	–3.626757	0.613459
6	4.610382	–1.864839	1.579416
1	5.387274	–1.296565	1.051316
1	5.009477	–2.038266	2.586111
6	–4.022038	–0.511984	–0.491175
1	–4.122068	0.115219	–1.392116
6	–4.832657	–1.792138	–0.777109
1	–5.905313	–1.555678	–0.840232
1	–4.566251	–2.144325	–1.779880
6	–4.656533	–2.950590	0.228975
1	–5.352496	–2.809441	1.059617
1	–4.976214	–3.885745	–0.248115
6	–3.239831	–3.136064	0.804872
1	–2.617230	–3.688193	0.090902
1	–3.313628	–3.791607	1.685182
6	–2.520204	–1.827921	1.170010
1	–1.516775	–2.105157	1.522404
6	–3.196326	–1.100740	2.349681
1	–3.360988	–1.800339	3.182950
1	–2.487527	–0.360293	2.735827
6	–4.530679	–0.395407	2.040164
1	–5.346673	–1.120147	2.100563
1	–4.741973	0.333472	2.833183
6	–4.597345	0.310047	0.676121

1	–4.037858	1.254528	0.729105
1	–5.644762	0.586798	0.482605
1	–1.948938	0.251093	0.227317
6	0.461065	1.417740	1.707108
6	–0.741810	1.780171	2.289756
6	1.652195	2.039864	2.049815
6	–0.744340	2.780426	3.252767
6	1.635269	3.037566	3.017151
6	0.439786	3.408996	3.620462
1	–1.651733	1.293124	1.966459
1	2.573645	1.755760	1.559250
1	–1.682501	3.068218	3.714127
1	2.563457	3.524512	3.296158
1	0.431430	4.186607	4.376364

PhOH

SCF energy = –307.425381035

8	2.294770	–0.109778	0.000161
1	2.674959	0.770760	0.000631
6	0.938680	–0.024242	–0.000345
6	0.263064	1.193303	–0.000116
6	0.220159	–1.217725	–0.000089
6	–1.127211	1.212832	0.000072
6	–1.165606	–1.184970	0.000110
6	–1.849425	0.027646	0.000012
1	0.819854	2.127545	–0.000109
1	0.764805	–2.155108	–0.000104
1	–1.644383	2.166768	0.000168
1	–1.717825	–2.119137	0.000154
1	–2.933537	0.046339	0.000103

3–BS

SCF energy = –2109.49734890

5	2.887239	–0.292868	–0.492504
16	0.923709	–0.672396	–1.208678
5	–3.108398	–0.057543	–0.437318
15	0.092151	0.730271	–0.043487
6	–0.649084	0.100020	1.496101
6	–0.267131	–1.147708	1.985149
1	0.355838	–1.795426	1.377749
6	–0.673302	–1.549800	3.250687
1	–0.374320	–2.521990	3.626435
6	–1.449385	–0.705227	4.035067
1	–1.760331	–1.019325	5.025710
6	–1.837021	0.538740	3.548574
1	–2.453675	1.193258	4.154563
6	–1.441237	0.942103	2.281331
1	–1.754643	1.909521	1.902893
6	1.488446	1.751230	0.441628
6	2.743075	1.193317	0.154771
6	3.837909	1.975819	0.565438
1	4.845218	1.622818	0.389922
6	3.682981	3.197638	1.201886
1	4.564024	3.762538	1.490984
6	2.416071	3.704979	1.479640
1	2.297810	4.659036	1.981663
6	1.309005	2.969575	1.101384
1	0.311007	3.348732	1.300873
6	–1.183190	1.747077	–0.839427
6	–2.536389	1.354618	–0.847132
6	–3.449618	2.253141	–1.411582
1	–4.506661	2.008165	–1.411404
6	–3.044833	3.448517	–1.994641
1	–3.783621	4.112124	–2.432085
6	–1.701678	3.791525	–2.014228
1	–1.373639	4.717132	–2.474010
6	–0.773621	2.945505	–1.422871
1	0.275381	3.219943	–1.415267
6	3.268877	–1.443611	0.587693
1	2.651452	–1.375363	1.495223
6	3.067720	–2.852116	–0.003932
1	3.425533	–3.612278	0.704285
1	1.990949	–3.028952	–0.113197
6	3.739459	–3.093096	–1.367280
1	3.319346	–4.001871	–1.813663
1	4.798978	–3.312806	–1.217677
6	3.598844	–1.934608	–2.368587
1	2.594846	–1.963077	–2.810056
1	4.287337	–2.110732	–3.206036
6	3.843325	–0.530524	–1.777838
1	3.637695	0.197968	–2.573466
6	5.320643	–0.340561	–1.363544
1	5.974097	–0.648138	–2.191194
1	5.508727	0.730441	–1.243114
6	5.766282	–1.092456	–0.090164
1	6.081926	–2.100814	–0.365223
1	6.670256	–0.614138	0.305929
6	4.723354	–1.191679	1.041380
1	4.739275	–0.270726	1.633910
1	5.039053	–1.985060	1.732184
6	–4.372301	–0.283902	0.471558
1	–4.631654	0.595148	1.073845

6	–5.562114	–0.549017	–0.498660
1	–6.433901	–0.869356	0.085194
1	–5.853028	0.402210	–0.959718
6	–5.285937	–1.568800	–1.617026
1	–5.418035	–2.583329	–1.239504
1	–6.043522	–1.449135	–2.398988
6	–3.893782	–1.437892	–2.247911
1	–3.866681	–0.542970	–2.884206
1	–3.712832	–2.284085	–2.920304
6	–2.718169	–1.357867	–1.222716
1	–1.800579	–1.261303	–1.809180
6	–2.586306	–2.601659	–0.322876
1	–2.554763	–3.504996	–0.944642
1	–1.606592	–2.543539	0.160396
6	–3.664317	–2.769563	0.761501
1	–4.537127	–3.277389	0.346176
1	–3.281166	–3.445339	1.533973
6	–4.105937	–1.462628	1.434034
1	–3.335650	–1.153267	2.144807
1	–5.005979	–1.653836	2.032019

3–BS1

SCF energy = –2267.90733095

5	–2.677693	–0.390169	–0.228519
16	–1.973732	0.634380	–2.030382
5	2.270108	–1.668027	–0.271854
15	0.454426	0.469723	0.688370
6	1.690803	1.756012	1.129128
6	2.679468	1.585131	2.096617
1	2.714427	0.668613	2.675694
6	3.626724	2.579850	2.319281
1	4.392459	2.431120	3.073775
6	3.594169	3.758089	1.585400
1	4.334481	4.531329	1.762095
6	2.610027	3.939903	0.618880
1	2.575612	4.856660	0.038693
6	1.675080	2.942025	0.389826
1	0.915685	3.088282	–0.372188
6	–1.111430	1.125506	1.417007
6	–2.380329	0.715060	0.932616
6	–3.484526	1.370767	1.498524
1	–4.478531	1.126003	1.143921
6	–3.379813	2.337287	2.489686
1	–4.275872	2.805458	2.885561
6	–2.130165	2.697314	2.966482
1	–2.023482	3.445114	3.745681
6	–1.006792	2.094645	2.421317
1	–0.028556	2.393509	2.781260
6	0.914052	–0.928763	1.780290
6	1.791302	–1.866980	1.212689
6	2.183095	–2.958213	1.992867
1	2.861262	–3.702814	1.584612
6	1.707346	–3.118925	3.289483
1	2.017532	–3.978978	3.874704
6	0.824042	–2.193032	3.830103
1	0.437759	–2.326703	4.835177
6	0.427994	–1.097107	3.073937
1	–0.272468	–0.377538	3.485829
6	–4.220966	–0.802433	–0.488487
1	–4.897174	0.062840	–0.535874
6	–4.408405	–1.553623	–1.820801
1	–5.452764	–1.878348	–1.918114
1	–4.246240	–0.848126	–2.644438
6	–3.494429	–2.771768	–2.022892
1	–3.499901	–3.048825	–3.083299
1	–3.918571	–3.632324	–1.502448
6	–2.039848	–2.561117	–1.572704
1	–1.500363	–2.045846	–2.378015
1	–1.550695	–3.540840	–1.488576
6	–1.835924	–1.770492	–0.263348
1	–0.756368	–1.624000	–0.170472
6	–2.267537	–2.550824	0.997109
1	–1.706081	–3.491937	1.062228
1	–1.971406	–1.967621	1.876645
6	–3.771393	–2.848801	1.080071
1	–4.012712	–3.696077	0.435070
1	–4.011582	–3.183770	2.095475
6	–4.670828	–1.649588	0.731152
1	–4.717258	–0.999113	1.610773
1	–5.696187	–2.008555	0.570549
6	3.505049	–0.786673	–0.681586
1	3.827895	–0.099436	0.107022
6	4.627741	–1.856325	–0.837279
1	5.559865	–1.359646	–1.132248
1	4.822865	–2.290087	0.153035
6	4.314533	–2.993415	–1.822980
1	4.448183	–2.638873	–2.845886
1	5.057382	–3.788007	–1.692634
6	2.908692	–3.594738	–1.657815
1	2.910084	–4.265553	–0.788909
1	2.675664	–4.231198	–2.520223
6	1.763905	–2.557202	–1.464844
1	0.856716	–3.120151	–1.221235

6	1.474336	–1.697754	–2.710200
1	1.222432	–2.344344	–3.560375
1	0.567372	–1.121204	–2.501005
6	2.589259	–0.725683	–3.120812
1	3.361080	–1.264940	–3.673363
1	2.180096	–0.002742	–3.835740
6	3.224735	0.041841	–1.950420
1	2.553496	0.858876	–1.658871
1	4.149122	0.523528	–2.293559
1	–0.685999	0.438013	–1.663932
6	–1.974279	2.432198	–1.723935
1	–2.969867	2.782148	–2.004121
1	–1.855653	2.592277	–0.651779
6	–0.885440	3.143885	–2.516469
1	0.077385	2.649628	–2.336274
1	–1.075963	3.047845	–3.590630
6	–0.772756	4.618982	–2.133242
1	–1.709936	5.132695	–2.375461
1	–0.653199	4.705792	–1.046664
6	0.394476	5.308292	–2.832134
1	1.345219	4.832980	–2.570089
1	0.291008	5.257094	–3.920003
1	0.461174	6.362866	–2.554057

3–BS2

SCF energy = –2267.89601361

5	–2.509716	–0.425616	–0.474475
16	–1.474375	0.589132	–1.880663
5	2.427775	–1.506628	–0.352528
15	0.281133	0.334301	1.106278
6	1.437899	1.661241	1.506487
6	2.420662	1.507843	2.481507
1	2.513458	0.569654	3.018624
6	3.297093	2.553089	2.744779
1	4.064119	2.434628	3.502179
6	3.195823	3.743063	2.034217
1	3.887126	4.553822	2.237671
6	2.212888	3.896759	1.061730
1	2.132399	4.824613	0.506207
6	1.331018	2.859484	0.798666
1	0.562895	2.981884	0.041910
6	–1.349734	0.809602	1.673781
6	–2.482119	0.514268	0.881983
6	–3.656892	1.146887	1.323226
1	–4.559644	1.026920	0.737384
6	–3.725351	1.929208	2.466192
1	–4.671063	2.382763	2.747458
6	–2.595635	2.145028	3.247817
1	–2.642388	2.751500	4.145633
6	–1.396397	1.601306	2.830041
1	–0.488260	1.814463	3.386847
6	0.907613	–1.213047	1.781914
6	1.851536	–1.949500	1.044386
6	2.262552	–3.170736	1.586544
1	2.965272	–3.789694	1.036750
6	1.780699	–3.623659	2.809440
1	2.125725	–4.573377	3.204805
6	0.836245	–2.884762	3.508778
1	0.433037	–3.253228	4.445288
6	0.384027	–1.681947	2.984209
1	–0.389115	–1.119785	3.498253
6	–4.020631	–0.809676	–0.972560
1	–4.642227	0.085845	–1.127349
6	–3.977690	–1.522032	–2.337036
1	–4.996090	–1.782134	–2.658644
1	–3.594580	–0.812591	–3.077139
6	–3.112649	–2.790310	–2.372892
1	–2.927613	–3.066253	–3.417874
1	–3.671292	–3.628797	–1.951320
6	–1.760554	–2.648513	–1.656205
1	–1.076297	–2.128985	–2.335078
1	–1.326949	–3.648466	–1.507997
6	–1.770726	–1.880473	–0.316321
1	–0.711207	–1.813912	–0.037903
6	–2.454035	–2.656156	0.824314
1	–1.957208	–3.624622	0.979872
1	–2.312526	–2.095229	1.758192
6	–3.955990	–2.895691	0.615185
1	–4.091026	–3.734656	–0.070074
1	–4.401154	–3.226144	1.561491
6	–4.733426	–1.668609	0.102862
1	–4.963646	–1.040301	0.969592
1	–5.706857	–2.008093	–0.278679
6	3.383348	–0.282241	–0.581605
1	3.483897	0.376806	0.285043
6	4.765526	–0.983144	–0.759092
1	5.533842	–0.214761	–0.905537
1	5.021387	–1.481122	0.186837
6	4.837452	–2.009677	–1.897833
1	4.901431	–1.488895	–2.853621
1	5.775044	–2.568777	–1.808024
6	3.663523	–3.002315	–1.917812
1	3.846095	–3.777199	–1.161508

1	3.640972	–3.528767	–2.879377
6	2.266304	–2.375383	–1.646950
1	1.550913	–3.195517	–1.520727
6	1.747560	–1.470233	–2.788447
1	1.668951	–2.056774	–3.711660
1	0.726459	–1.164664	–2.542352
6	2.564807	–0.201315	–3.057030
1	3.462071	–0.443422	–3.630113
1	1.971963	0.454681	–3.702359
6	2.941449	0.575963	–1.786603
1	2.068354	1.162924	–1.475062
1	3.721188	1.311984	–2.018962
1	0.160277	0.278518	–0.312770
6	–1.779185	2.354026	–1.539279
1	–2.827330	2.584036	–1.749920
1	–1.627426	2.555734	–0.473233
6	–0.861904	3.241344	–2.372082
1	0.181048	2.929682	–2.223499
1	–1.066163	3.082861	–3.436654
6	–1.004539	4.724209	–2.032846
1	–2.041078	5.036766	–2.204083
1	–0.821089	4.875160	–0.960707
6	–0.060899	5.607636	–2.842826
1	0.985964	5.350117	–2.650302
1	–0.233826	5.485915	–3.916244
1	–0.193151	6.666273	–2.603638

3–BS3

SCF energy = –2267.87182777

5	–2.624037	–1.032576	0.093080
16	–0.550771	0.853749	–1.193482
5	2.521937	–0.800700	–0.499097
15	0.274631	0.453708	0.727859
6	1.345372	1.814182	1.285611
6	2.224471	1.591426	2.343716
1	2.270190	0.617441	2.818255
6	3.062269	2.612709	2.772889
1	3.754458	2.430357	3.587617
6	3.027578	3.853395	2.149552
1	3.689676	4.646078	2.481113
6	2.154135	4.073408	1.091265
1	2.133911	5.036099	0.592188
6	1.315156	3.056856	0.656997
1	0.661636	3.227220	–0.191259
6	–1.288783	0.661280	1.705049
6	–2.447244	–0.060329	1.337568
6	–3.577722	0.100194	2.147359
1	–4.496973	–0.414773	1.887866
6	–3.572718	0.903662	3.282418
1	–4.469286	0.988712	3.887944
6	–2.430906	1.611199	3.617653
1	–2.417229	2.259664	4.487294
6	–1.296935	1.494130	2.820953
1	–0.409720	2.060397	3.081246
6	0.854048	–1.142337	1.385037
6	1.975341	–1.664166	0.731854
6	2.502334	–2.851122	1.261973
1	3.369973	–3.305962	0.796436
6	1.938054	–3.463654	2.370862
1	2.366502	–4.385878	2.752205
6	0.829237	–2.905948	3.006439
1	0.395527	–3.384341	3.877995
6	0.279061	–1.735843	2.514073
1	–0.591238	–1.305573	2.994013
6	–3.880044	–0.901868	–0.864964
1	–4.409684	0.052801	–0.750312
6	–3.434228	–1.026588	–2.336814
1	–4.315257	–0.990463	–2.990413
1	–2.836567	–0.144469	–2.593498
6	–2.625165	–2.292536	–2.655052
1	–2.143496	–2.166084	–3.630210
1	–3.314120	–3.130166	–2.783764
6	–1.545946	–2.651112	–1.617452
1	–0.648422	–2.063143	–1.829478
1	–1.251069	–3.698736	–1.756205
6	–1.901478	–2.409908	–0.135107
1	–0.987480	–2.538325	0.443026
6	–2.930189	–3.423707	0.445813
1	–2.495580	–4.428999	0.403996
1	–3.074477	–3.206148	1.513403
6	–4.289383	–3.420087	–0.260901
1	–4.194282	–3.919249	–1.226017
1	–4.994725	–4.029937	0.314069
6	–4.886383	–2.015825	–0.446952
1	–5.362683	–1.716545	0.494057
1	–5.697071	–2.055372	–1.185022
6	3.952573	–0.070177	–0.329383
1	4.069500	0.379392	0.666129
6	5.065397	–1.129425	–0.469572
1	6.053527	–0.648838	–0.441637
1	5.029772	–1.770442	0.420716
6	4.986376	–2.019107	–1.724586
1	5.424910	–1.489503	–2.573020

1	5.626566	–2.897437	–1.577098
6	3.570632	–2.491206	–2.101582
1	3.287822	–3.332082	–1.455749
1	3.598603	–2.903475	–3.119951
6	2.469349	–1.416295	–1.992072
1	1.515634	–1.922650	–2.195525
6	2.609443	–0.282973	–3.025802
1	2.667807	–0.698346	–4.042045
1	1.686954	0.308836	–2.995721
6	3.799781	0.669485	–2.813332
1	4.708878	0.218963	–3.218851
1	3.639236	1.574106	–3.412403
6	4.040876	1.077826	–1.351215
1	3.291024	1.828070	–1.067365
1	5.014280	1.584052	–1.281059
1	1.606834	0.142842	–0.444486
6	–1.883742	2.097324	–0.927501
1	–1.665025	2.670597	–0.025686
1	–2.834236	1.589170	–0.771037
6	–1.947247	3.007910	–2.147487
1	–0.979980	3.502539	–2.291771
1	–2.124934	2.412460	–3.050617
6	–3.050168	4.056365	–2.003727
1	–4.014997	3.553543	–1.870756
1	–2.879881	4.637111	–1.089454
6	–3.120169	4.995007	–3.203805
1	–2.174835	5.527759	–3.343812
1	–3.327278	4.443982	–4.125922
1	–3.907512	5.742648	–3.080157

nBuSH

SCF energy = –556.629134845

16	–2.355491	–0.202164	–0.081872
1	–2.226376	–0.934928	1.040907
6	–0.749027	0.657151	0.050808
1	–0.746027	1.360751	–0.785691
1	–0.738545	1.252189	0.966885
6	0.463727	–0.261067	–0.021149
1	0.427166	–0.981036	0.805784
1	0.414915	–0.850730	–0.942886
6	1.782018	0.510180	0.035664
1	1.817692	1.229635	–0.790992
1	1.818989	1.103153	0.957450
6	2.999453	–0.406666	–0.031106
1	3.003791	–1.118982	0.799479
1	3.007231	–0.984448	–0.960286
1	3.931984	0.161439	0.013996

3–BCN1

SCF energy = –1961.93024926

15	–0.180104	1.110763	–0.198054
7	2.141639	–0.180627	2.367023
6	–0.938403	2.712098	0.320271
6	–0.187430	3.535426	1.163532
1	0.840513	3.269443	1.394600
6	–0.711002	4.717003	1.659240
1	–0.100691	5.347666	2.294912
6	–2.009788	5.096588	1.332795
1	–2.422067	6.021710	1.717091
6	–2.768729	4.286254	0.504448
1	–3.780276	4.576254	0.235770
6	–2.239105	3.103911	–0.000107
1	–2.846032	2.496008	–0.659249
6	1.409861	1.693396	–0.948700
6	2.554531	0.863923	–0.920636
6	3.737146	1.423197	–1.426668
1	4.654725	0.848856	–1.380074
6	3.799055	2.695209	–1.977034
1	4.741533	3.074393	–2.361207
6	2.655437	3.478988	–2.028890
1	2.681192	4.473488	–2.463010
6	1.475298	2.977380	–1.504684
1	0.585115	3.597360	–1.524250
6	–1.215884	0.677122	–1.671382
6	–2.454950	0.006368	–1.503421
6	–3.276195	–0.106156	–2.640709
1	–4.254505	–0.563050	–2.545392
6	–2.881143	0.318876	–3.900182
1	–3.544276	0.192086	–4.751323
6	–1.632165	0.897591	–4.054607
1	–1.291022	1.222544	–5.031909
6	–0.820484	1.090371	–2.942994
1	0.138702	1.573986	–3.077859
6	1.485493	–1.730196	–0.868408
1	0.469811	–1.324629	–0.844425
6	1.798376	–1.989929	–2.350068
1	1.046235	–2.666805	–2.777698
1	1.689381	–1.038918	–2.886938
6	3.195013	–2.561567	–2.619658
1	3.404524	–2.504322	–3.694031
1	3.204704	–3.628258	–2.384078
6	4.319773	–1.839728	–1.859745

1	4.556093	–0.924206	–2.410897
1	5.230049	–2.453738	–1.902782
6	4.019440	–1.469151	–0.389972
1	4.858903	–0.849935	–0.041900
6	3.983240	–2.702814	0.532335
1	4.926222	–3.259892	0.453207
1	3.937310	–2.357647	1.574870
6	2.817154	–3.671833	0.276412
1	2.715557	–4.344511	1.136450
1	3.072951	–4.323074	–0.561457
6	1.459133	–2.999637	0.005274
1	0.785529	–3.744566	–0.437067
1	0.999136	–2.732869	0.968161
6	–2.045584	–1.677027	0.692379
1	–0.997241	–1.373549	0.699985
6	–2.102625	–3.046302	–0.048444
1	–1.632505	–2.909804	–1.029010
1	–1.470475	–3.764699	0.482597
6	–3.510289	–3.636368	–0.231673
1	–3.820909	–4.133071	0.683378
1	–3.455733	–4.428634	–0.979848
6	–4.582684	–2.626339	–0.677832
1	–5.581570	–3.038193	–0.480579
1	–4.511972	–2.519452	–1.763572
6	–4.479602	–1.200629	–0.052523
1	–5.174005	–0.558257	–0.604888
6	–4.909789	–1.158573	1.425377
1	–4.908168	–0.114170	1.761602
1	–5.950565	–1.499471	1.513224
6	–4.025551	–1.981743	2.361642
1	–4.248658	–3.039779	2.234644
1	–4.286587	–1.753987	3.397692
6	–2.528023	–1.727229	2.153522
1	–1.950810	–2.481911	2.702920
1	–2.282831	–0.764038	2.615643
6	2.303880	–0.399468	1.245374
6	1.736121	0.101660	3.724431
6	0.238663	–0.203727	3.808776
1	–0.318777	0.406455	3.093583
1	–0.124206	0.013844	4.816895
1	0.044110	–1.255362	3.584955
6	2.012363	1.581295	4.002439
1	1.401868	2.212235	3.352986
1	3.067972	1.820413	3.844575
1	1.756038	1.810361	5.042272
6	2.555651	–0.801377	4.648367
1	2.357546	–1.861241	4.427367
1	2.273414	–0.599134	5.690024
1	3.636221	–0.614891	4.534208
5	2.589244	–0.658392	–0.295927
5	–2.954965	–0.799463	–0.241707

3–BCN2

SCF energy = –2212.61396156

15	0.228131	0.877767	–0.661281
7	1.729506	0.657086	2.670840
7	–3.454183	0.338473	0.584588
6	–0.886441	2.351012	–0.815092
6	–0.589416	3.475389	–0.033698
1	0.311830	3.480306	0.572894
6	–1.390466	4.607114	–0.066137
1	–1.126358	5.472085	0.534074
6	–2.523866	4.635994	–0.874441
1	–3.151371	5.520670	–0.906498
6	–2.831209	3.527951	–1.652564
1	–3.698657	3.546282	–2.305195
6	–2.019297	2.396196	–1.626377
1	–2.261505	1.552144	–2.263436
6	1.831338	1.702077	–1.115580
6	3.048733	1.308130	–0.516492
6	4.168242	2.105319	–0.800440
1	5.111344	1.879618	–0.316977
6	4.130666	3.184932	–1.669645
1	5.032576	3.759957	–1.858211
6	2.938272	3.520873	–2.294695
1	2.887660	4.351471	–2.991629
6	1.800302	2.788900	–2.001377
1	0.863244	3.075242	–2.466891
6	–0.259943	–0.087240	–2.165838
6	–1.363201	–0.978580	–2.129081
6	–1.834531	–1.409589	–3.378168
1	–2.729890	–2.016606	–3.421560
6	–1.208421	–1.109434	–4.580090
1	–1.616028	–1.490359	–5.511717
6	–0.053565	–0.345528	–4.574536
1	0.479579	–0.131127	–5.495246
6	0.395846	0.177724	–3.371959
1	1.272804	0.812585	–3.378169
6	2.661727	–1.420315	–0.109154
1	1.627412	–1.338544	–0.457048
6	3.499014	–1.786000	–1.343625
1	3.111561	–2.709576	–1.794197
1	3.354966	–1.000568	–2.096237

6	4.998270	–1.952634	–1.069848
1	5.534764	–1.995636	–2.024432
1	5.174722	–2.922417	–0.598611
6	5.606520	–0.828398	–0.213083
1	5.804790	0.019237	–0.875718
1	6.590137	–1.154048	0.152424
6	4.753856	–0.337919	0.979398
1	5.258138	0.550487	1.386090
6	4.703036	–1.365444	2.125764
1	5.720770	–1.611262	2.457189
1	4.220902	–0.896699	2.995572
6	3.968992	–2.670887	1.786145
1	3.752343	–3.213142	2.714543
1	4.645463	–3.322170	1.229736
6	2.661810	–2.499142	0.991556
1	2.395122	–3.469823	0.558030
1	1.847833	–2.262796	1.692458
6	–1.100141	–2.289979	0.337627
1	–0.304126	–1.601374	0.640802
6	–0.414811	–3.495571	–0.325062
1	0.204883	–3.122431	–1.149052
1	0.277628	–3.960727	0.385969
6	–1.364711	–4.576448	–0.854356
1	–1.702103	–5.201558	–0.024450
1	–0.801534	–5.251838	–1.507891
6	–2.572698	–4.032322	–1.632650
1	–3.327561	–4.826261	–1.718067
1	–2.242926	–3.829572	–2.653988
6	–3.238072	–2.761990	–1.055045
1	–3.983989	–2.430845	–1.791419
6	–4.024786	–3.072187	0.233004
1	–4.621428	–2.190630	0.504828
1	–4.758543	–3.865763	0.039308
6	–3.161829	–3.485302	1.434950
1	–2.905192	–4.541611	1.342680
1	–3.762463	–3.417404	2.350529
6	–1.879055	–2.655767	1.618582
1	–1.217085	–3.185698	2.317698
1	–2.152853	–1.723948	2.130003
6	2.362454	0.380333	1.745566
6	0.734185	0.873489	3.692442
6	–0.428656	–0.064421	3.367038
1	–0.807070	0.139158	2.363550
1	–1.232861	0.076562	4.094614
1	–0.111924	–1.108150	3.399444
6	0.295684	2.336924	3.619334
1	–0.150509	2.558401	2.648464
1	1.140831	3.009201	3.779321
1	–0.450475	2.530273	4.393965
6	1.367344	0.544280	5.044337
1	1.720441	–0.488706	5.065051
1	0.624209	0.671664	5.835030
1	2.211870	1.203694	5.252523
6	–2.854850	–0.428124	–0.035777
6	–4.271676	1.171457	1.434658
6	–4.843437	0.258486	2.523502
1	–5.454074	–0.537710	2.091513
1	–5.467185	0.847866	3.199436
1	–4.037826	–0.201174	3.101773
6	–5.378196	1.777314	0.570745
1	–4.950372	2.401998	–0.214840
1	–6.024841	2.398629	1.194925
1	–5.986728	0.995800	0.111409
6	–3.380348	2.257850	2.034538
1	–2.938808	2.878318	1.254340
1	–2.575686	1.815621	2.626280
1	–3.981407	2.894349	2.688544
5	3.227986	0.009435	0.472031
5	–2.089925	–1.595036	–0.783743

3–BCO

SCF energy = –1824.60040984

5	–1.950862	0.531983	–0.414704
5	0.026874	–1.555217	0.686281
15	1.192721	0.795690	0.133701
6	2.953174	1.015550	–0.181370
6	3.382845	1.383916	–1.459131
1	2.658759	1.630370	–2.228627
6	4.739054	1.435067	–1.742139
1	5.071797	1.717987	–2.734659
6	5.668721	1.121461	–0.755749
1	6.729241	1.161840	–0.980049
6	5.243319	0.757715	0.515574
1	5.968409	0.512340	1.283480
6	3.886013	0.700231	0.805664
1	3.552230	0.401677	1.793673
6	0.239619	2.160167	–0.503275
6	–1.133401	1.921542	–0.734727
6	–1.825639	3.052637	–1.205011
1	–2.882023	2.975866	–1.408943
6	–1.229795	4.288338	–1.405817
1	–1.833863	5.116689	–1.763341
6	0.122822	4.477199	–1.149896

1	0.592330	5.443060	–1.300971
6	0.859669	3.400623	–0.695204
1	1.918651	3.522209	–0.489787
6	0.858666	0.507597	1.872292
6	0.262291	–0.747616	2.046110
6	–0.102287	–1.099665	3.344662
1	–0.571678	–2.061372	3.528800
6	0.104170	–0.221748	4.402118
1	–0.193317	–0.508115	5.406056
6	0.673115	1.033411	4.190639
1	0.815757	1.714094	5.023000
6	1.050852	1.412714	2.910609
1	1.485891	2.391342	2.730231
6	–3.060852	0.053682	–1.513577
1	–2.651051	0.060390	–2.534587
6	–3.479381	–1.393699	–1.200631
1	–4.240692	–1.725409	–1.920081
1	–2.619726	–2.043091	–1.354920
6	–4.027104	–1.599785	0.220240
1	–4.063163	–2.674720	0.436570
1	–5.068884	–1.271718	0.252746
6	–3.229003	–0.897523	1.335075
1	–2.367433	–1.524988	1.584718
1	–3.842370	–0.874192	2.246761
6	–2.715999	0.524281	1.016351
1	–2.049195	0.815610	1.839543
6	–3.842727	1.573924	0.973321
1	–4.376951	1.587226	1.932924
1	–3.384532	2.565359	0.882515
6	–4.877066	1.378202	–0.150214
1	–5.605410	0.633737	0.177686
1	–5.453022	2.304142	–0.266479
6	–4.316261	0.960942	–1.529519
1	–4.115285	1.851486	–2.130285
1	–5.115534	0.444770	–2.078500
6	1.110367	–1.395424	–1.798039
1	1.399002	–0.609041	–2.511128
6	2.405567	–2.170661	–1.473391
1	2.909558	–2.387192	–2.423524
1	3.080343	–1.489769	–0.943214
6	2.337339	–3.492017	–0.682601
1	1.993836	–4.289662	–1.342101
1	3.375045	–3.757747	–0.446122
6	1.544191	–3.560839	0.633230
1	2.062451	–2.956819	1.391303
1	1.621594	–4.597613	0.986749
6	0.054672	–3.140066	0.607318
1	–0.376958	–3.529012	1.542207
6	–0.782706	–3.792004	–0.505073
1	–0.777084	–4.879683	–0.350043
1	–1.818314	–3.487476	–0.338419
6	–0.426614	–3.572073	–1.992350
1	0.328666	–4.303563	–2.285176
1	–1.313845	–3.852401	–2.572557
6	0.010834	–2.193947	–2.523951
1	–0.858739	–1.539407	–2.609511
1	0.363880	–2.356372	–3.549207
6	0.573806	–0.746483	–0.535492
8	–0.851611	–0.720489	–0.332050

3–BCTS1

SCF energy = –1824.57436139

5	–2.879244	–0.330980	–0.181088
5	1.833914	–1.126101	–0.124806
15	–0.048498	1.205366	–0.254513
6	1.184922	2.533984	–0.091605
6	1.795904	3.008345	–1.252699
1	1.520657	2.595706	–2.218742
6	2.771100	3.994602	–1.175470
1	3.246942	4.355679	–2.080729
6	3.145302	4.503897	0.061763
1	3.914398	5.266509	0.123316
6	2.542556	4.029858	1.222354
1	2.841061	4.421873	2.188773
6	1.564625	3.047908	1.148186
1	1.111217	2.662525	2.055535
6	–1.676475	2.030206	–0.269402
6	–2.839481	1.240980	–0.150197
6	–4.065084	1.910833	–0.069962
1	–4.977407	1.337050	0.061781
6	–4.154603	3.294519	–0.169985
1	–5.123942	3.779957	–0.124288
6	–3.000777	4.050139	–0.312635
1	–3.057215	5.131275	–0.382775
6	–1.762675	3.419870	–0.343375
1	–0.861745	4.019027	–0.416500
6	0.013765	0.215841	1.245655
6	0.877328	–0.900384	1.180341
6	0.898414	–1.699172	2.332564
1	1.529918	–2.575603	2.363877
6	0.146723	–1.404425	3.462807
1	0.205228	–2.059067	4.327030
6	–0.682026	–0.288842	3.495060

1	–1.271736	–0.060555	4.376426
6	–0.752501	0.520204	2.374123
1	–1.412576	1.382304	2.367019
6	–2.357032	–1.171314	–1.400334
1	–1.706883	–0.610073	–2.079016
6	–1.625638	–2.460205	–0.974529
1	–1.473404	–3.108610	–1.846293
1	–0.625148	–2.176783	–0.638232
6	–2.278985	–3.264613	0.160574
1	–1.521256	–3.926593	0.593566
1	–3.047868	–3.929984	–0.237133
6	–2.870040	–2.401515	1.281730
1	–2.050855	–2.007229	1.891190
1	–3.464668	–3.037111	1.950064
6	–3.731580	–1.210773	0.804306
1	–4.063339	–0.656337	1.690228
6	–5.005448	–1.640026	0.019596
1	–5.559347	–2.381409	0.608870
1	–5.670064	–0.770745	–0.058067
6	–4.756869	–2.187851	–1.396849
1	–4.485807	–3.243176	–1.349004
1	–5.697319	–2.155002	–1.957531
6	–3.684061	–1.421798	–2.181925
1	–4.092132	–0.451656	–2.496887
1	–3.450904	–1.960576	–3.107680
6	3.259052	–0.298940	0.006488
1	3.097739	0.746894	0.290158
6	4.039090	–0.941715	1.168673
1	4.988436	–0.407753	1.309048
1	3.470690	–0.781286	2.091728
6	4.345322	–2.438952	1.011005
1	5.212944	–2.553601	0.357871
1	4.665705	–2.839258	1.979917
6	3.186744	–3.301767	0.473288
1	2.568940	–3.642950	1.306946
1	3.610815	–4.223025	0.051858
6	2.282180	–2.641893	–0.594065
1	1.410704	–3.299315	–0.716794
6	3.013305	–2.600298	–1.952856
1	3.354252	–3.611787	–2.209912
1	2.306603	–2.324820	–2.739059
6	4.226862	–1.654333	–2.006050
1	5.090170	–2.154299	–1.561814
1	4.500928	–1.490546	–3.054373
6	4.029622	–0.285493	–1.326508
1	3.499769	0.380680	–2.019678
1	5.014236	0.178026	–1.179445
6	1.060631	–0.445024	–1.404250
8	0.945666	–0.433068	–2.552372

3–BCTS2

SCF energy = –1824.56598452

5	–2.563731	–0.131737	–0.499498
5	1.505057	–1.296706	–0.052669
15	0.280782	1.240709	0.318397
6	1.613057	2.354673	–0.172262
6	1.622550	2.866406	–1.470913
1	0.819976	2.625366	–2.161052
6	2.665630	3.683295	–1.879605
1	2.680454	4.073102	–2.891307
6	3.691274	3.998330	–0.994084
1	4.506231	4.637028	–1.317367
6	3.677479	3.494331	0.300537
1	4.478975	3.736946	0.989362
6	2.642332	2.666264	0.713643
1	2.647390	2.241986	1.711929
6	–1.262268	2.129728	0.088270
6	–2.383688	1.456679	–0.447716
6	–3.448693	2.277756	–0.842244
1	–4.316398	1.823538	–1.303960
6	–3.443261	3.653146	–0.659263
1	–4.302816	4.239692	–0.967883
6	–2.341341	4.281425	–0.092697
1	–2.330413	5.355500	0.056800
6	–1.238284	3.520230	0.251200
1	–0.348989	4.009652	0.635186
6	0.691026	0.389196	1.827935
6	1.276106	–0.865549	1.531222
6	1.608109	–1.633142	2.655526
1	2.054949	–2.609547	2.520008
6	1.380096	–1.182323	3.949065
1	1.655488	–1.814619	4.787744
6	0.795434	0.059508	4.191651
1	0.611451	0.392596	5.207163
6	0.442488	0.856526	3.116997
1	–0.035030	1.819474	3.273205
6	–3.548510	–0.872690	–1.505924
1	–3.586922	–0.392433	–2.492544
6	–3.081034	–2.329889	–1.711088
1	–3.798594	–2.856157	–2.353848
1	–2.135878	–2.315962	–2.258109
6	–2.901578	–3.140213	–0.415045
1	–2.311169	–4.034482	–0.643704

1	–3.874773	–3.518642	–0.093380
6	–2.224230	–2.395191	0.752668
1	–1.141329	–2.478092	0.639461
1	–2.458651	–2.916840	1.689834
6	–2.560421	–0.899510	0.897064
1	–1.859004	–0.475633	1.626845
6	–3.980288	–0.636171	1.459966
1	–4.062566	–1.077782	2.460612
1	–4.113151	0.445347	1.596240
6	–5.112617	–1.177819	0.578151
1	–5.165905	–2.261686	0.693112
1	–6.070022	–0.799989	0.954398
6	–4.985038	–0.811521	–0.911587
1	–5.390137	0.196405	–1.049479
1	–5.640154	–1.466732	–1.499693
6	2.939686	–0.755947	–0.646074
1	3.129393	0.295485	–0.406954
6	4.070100	–1.546414	0.034733
1	5.045274	–1.190133	–0.325191
1	4.044726	–1.311378	1.107079
6	4.008228	–3.069458	–0.145179
1	4.389534	–3.326401	–1.135791
1	4.705946	–3.539362	0.558139
6	2.610721	–3.686200	0.047050
1	2.448395	–3.867620	1.114410
1	2.604903	–4.685223	–0.410150
6	1.426474	–2.863795	–0.503312
1	0.514676	–3.352395	–0.135644
6	1.360563	–2.919215	–2.044345
1	1.321612	–3.964501	–2.380326
1	0.416346	–2.469111	–2.366339
6	2.524168	–2.220075	–2.766971
1	3.395709	–2.878758	–2.770109
1	2.262613	–2.090385	–3.823675
6	2.921413	–0.852702	–2.183290
1	2.211366	–0.097015	–2.552215
1	3.897595	–0.562303	–2.596003
6	0.256873	–0.427471	–0.634911
8	–0.761849	–0.677566	–1.239617

3–BCTS3

SCF energy = –1824.55659656

5	–2.054165	0.556231	–0.544489
5	1.909503	1.068946	–0.788028
15	0.473106	–1.161870	–0.166579
6	0.224564	–2.010276	1.412886
6	–0.903989	–2.801800	1.625707
1	–1.657453	–2.892308	0.850869
6	–1.066268	–3.457797	2.838176
1	–1.947585	–4.067235	3.003614
6	–0.109288	–3.324716	3.836973
1	–0.243701	–3.832298	4.786159
6	1.023056	–2.546924	3.621667
1	1.775521	–2.451316	4.396587
6	1.196392	–1.895259	2.409436
1	2.094601	–1.311495	2.236115
6	–0.759306	–1.641725	–1.367772
6	–1.849737	–0.759630	–1.516568
6	–2.738552	–1.113809	–2.541555
1	–3.582169	–0.469277	–2.748464
6	–2.576324	–2.251097	–3.320389
1	–3.299925	–2.472531	–4.099160
6	–1.492802	–3.102183	–3.125587
1	–1.363428	–3.987390	–3.738663
6	–0.566506	–2.784480	–2.149161
1	0.308125	–3.411890	–2.006006
6	2.166792	–1.459285	–0.647943
6	2.812859	–0.250639	–0.950422
6	4.130587	–0.356672	–1.403463
1	4.681819	0.531100	–1.686933
6	4.760026	–1.591793	–1.512569
1	5.781626	–1.640784	–1.875970
6	4.103163	–2.764391	–1.152833
1	4.609367	–3.720774	–1.224912
6	2.789402	–2.700744	–0.711437
1	2.262260	–3.604272	–0.420066
6	–2.564450	0.152716	0.954347
1	–1.938962	–0.601298	1.441394
6	–2.545903	1.367822	1.903991
1	–3.097548	1.126890	2.824052
1	–1.510767	1.510918	2.228907
6	–3.086427	2.703633	1.347457
1	–2.641746	3.528214	1.918487
1	–4.158791	2.770766	1.547765
6	–2.852839	2.951127	–0.153816
1	–1.830678	3.303732	–0.316643
1	–3.510130	3.772312	–0.471773
6	–3.087634	1.711174	–1.038893
1	–2.876449	2.013068	–2.075475
6	–4.570848	1.269772	–0.988432
1	–5.216890	2.151731	–1.100244
1	–4.797113	0.649900	–1.861137

6	–5.013296	0.496832	0.268998
1	–5.282685	1.198543	1.062017
1	–5.936363	–0.050969	0.045099
6	–3.963176	–0.475950	0.816020
1	–3.900170	–1.350118	0.153505
1	–4.309000	–0.856377	1.787518
6	1.461857	1.476068	1.141892
1	0.983602	0.775017	1.829895
6	2.958792	1.502549	1.537489
1	2.977733	1.605366	2.630935
1	3.434623	0.541359	1.325603
6	3.793466	2.656665	0.962550
1	3.500845	3.569541	1.484962
1	4.836845	2.486414	1.248479
6	3.726665	2.884467	–0.563657
1	4.546598	2.336184	–1.031313
1	3.944228	3.940919	–0.763373
6	2.396933	2.502781	–1.262841
1	2.619794	2.416067	–2.336008
6	1.325944	3.593357	–1.104767
1	1.637099	4.493235	–1.650396
1	0.392027	3.254968	–1.560321
6	1.076059	3.985855	0.352010
1	1.934495	4.554962	0.717583
1	0.232755	4.683267	0.390691
6	0.750002	2.822793	1.306057
1	–0.316325	2.635425	1.237088
1	0.930201	3.147619	2.339411
6	0.502366	0.684215	–0.376755
8	–0.643631	1.273631	–0.504924

3–BCTS4

SCF energy = –1824.58910492

5	1.992951	–0.496119	–0.517849
5	–0.352874	1.709977	0.696041
15	–1.045758	–0.834963	0.117076
6	–2.798399	–1.170977	–0.173604
6	–3.206265	–1.556882	–1.453710
1	–2.469323	–1.730423	–2.230825
6	–4.554215	–1.728550	–1.728176
1	–4.866656	–2.026279	–2.723028
6	–5.501088	–1.519975	–0.730641
1	–6.555177	–1.655733	–0.947460
6	–5.098472	–1.142633	0.544023
1	–5.835576	–0.983486	1.323385
6	–3.749674	–0.964274	0.824571
1	–3.440436	–0.656529	1.817554
6	–0.072549	–2.210359	–0.458805
6	1.283594	–1.957495	–0.756595
6	1.983235	–3.086158	–1.218044
1	3.024632	–2.979830	–1.483442
6	1.408633	–4.341162	–1.339494
1	2.011568	–5.171914	–1.694226
6	0.071813	–4.548657	–1.011342
1	–0.380034	–5.530498	–1.102252
6	–0.674471	–3.472225	–0.574543
1	–1.722963	–3.609111	–0.329441
6	–0.806219	–0.444613	1.859214
6	–0.473312	0.907001	2.035681
6	–0.229775	1.353875	3.335569
1	0.042783	2.390605	3.506727
6	–0.302120	0.472818	4.405502
1	–0.096785	0.823831	5.411369
6	–0.618367	–0.869695	4.198259
1	–0.652895	–1.552274	5.040695
6	–0.874617	–1.341340	2.917944
1	–1.099290	–2.389794	2.749381
6	3.265654	–0.116352	–1.483733
1	3.006483	–0.258364	–2.543784
6	3.567421	1.382658	–1.292029
1	4.412305	1.683149	–1.928358
1	2.705907	1.956172	–1.640513
6	3.895486	1.769716	0.160329
1	3.847720	2.861530	0.262952
1	4.937998	1.515383	0.367145
6	2.990013	1.133735	1.234028
1	2.073181	1.733194	1.297571
1	3.473061	1.247219	2.215787
6	2.578032	–0.334473	1.005676
1	1.829952	–0.571491	1.775136
6	3.723550	–1.339491	1.219504
1	4.098889	–1.277429	2.250936
1	3.312002	–2.351689	1.115071
6	4.913840	–1.176135	0.263917
1	5.533853	–0.348860	0.617436
1	5.556849	–2.061846	0.337546
6	4.543892	–0.946259	–1.215957
1	4.462639	–1.916790	–1.713576
1	5.397647	–0.462438	–1.711762
6	–1.184901	1.338941	–1.776676
1	–1.421350	0.507410	–2.455553
6	–2.539338	1.950628	–1.348925
1	–3.209082	1.908630	–2.215305

1	–3.011962	1.301556	–0.603832
6	–2.583699	3.392388	–0.821479
1	–2.319659	4.076590	–1.627093
1	–3.634589	3.612724	–0.599287
6	–1.775854	3.735210	0.441779
1	–2.310230	3.335496	1.314794
1	–1.795611	4.825007	0.565438
6	–0.297474	3.260642	0.526214
1	0.091386	3.696834	1.457405
6	0.632029	3.764947	–0.595772
1	0.811369	4.835316	–0.431088
1	1.599941	3.277758	–0.462763
6	0.194699	3.621914	–2.062564
1	–0.560292	4.381473	–2.274967
1	1.056808	3.917700	–2.671354
6	–0.274466	2.258694	–2.612824
1	0.604165	1.662441	–2.862137
1	–0.793122	2.452973	–3.559726
6	–0.407818	0.767550	–0.572471
8	0.949636	0.616109	–0.841327

3–BCI1

SCF energy = –1824.57867856

5	–3.023479	–0.279057	–0.131525
5	2.027647	–1.361397	–0.155078
15	–0.038528	1.167730	–0.532501
6	1.147719	2.539911	–0.208764
6	1.655868	3.229011	–1.312726
1	1.329000	2.955112	–2.312003
6	2.584174	4.248546	–1.147521
1	2.971152	4.772806	–2.015146
6	3.028499	4.582249	0.126757
1	3.764596	5.368631	0.257855
6	2.533774	3.898631	1.230675
1	2.882231	4.150157	2.227140
6	1.596240	2.886331	1.065031
1	1.224062	2.353152	1.933096
6	–1.669316	2.021049	–0.325355
6	–2.866582	1.285626	–0.148623
6	–4.057865	2.010426	–0.007956
1	–4.984576	1.474931	0.172413
6	–4.105731	3.395452	–0.100419
1	–5.053128	3.916452	–0.008311
6	–2.928051	4.098442	–0.287830
1	–2.935900	5.182211	–0.346570
6	–1.721073	3.414619	–0.378268
1	–0.807752	3.987466	–0.485683
6	0.090905	0.145181	1.000510
6	0.936269	–0.989951	1.013258
6	0.833185	–1.829477	2.129345
1	1.395892	–2.754430	2.153461
6	0.021148	–1.541678	3.218683
1	–0.017950	–2.228106	4.058688
6	–0.734440	–0.380294	3.224413
1	–1.361283	–0.127198	4.073262
6	–0.708739	0.443766	2.108712
1	–1.334257	1.329394	2.095613
6	–2.429900	–1.261822	–1.205987
1	–1.637448	–0.816198	–1.813871
6	–1.896543	–2.572142	–0.590546
1	–1.677729	–3.296879	–1.385568
1	–0.939089	–2.343776	–0.112617
6	–2.781438	–3.234965	0.476326
1	–2.163853	–3.931535	1.054085
1	–3.549542	–3.852640	0.007097
6	–3.433872	–2.241316	1.443814
1	–2.670655	–1.879145	2.140955
1	–4.178260	–2.768230	2.054383
6	–4.089451	–1.017227	0.769827
1	–4.488779	–0.376060	1.564868
6	–5.278029	–1.388760	–0.164179
1	–5.980540	–2.030641	0.382155
1	–5.831896	–0.470532	–0.394465
6	–4.891998	–2.061211	–1.493437
1	–4.740770	–3.131024	–1.343898
1	–5.735950	–1.983053	–2.187487
6	–3.647214	–1.459345	–2.158356
1	–3.905983	–0.485619	–2.594925
1	–3.340541	–2.091607	–3.000359
6	3.126792	–0.201905	–0.571711
1	2.643064	0.744272	–0.808807
6	3.985025	0.055176	0.676258
1	4.682936	0.877481	0.473928
1	3.324294	0.411273	1.475657
6	4.770953	–1.164610	1.167637
1	5.646203	–1.312050	0.532008
1	5.173064	–0.956503	2.165045
6	3.939529	–2.456902	1.236272
1	3.381724	–2.440674	2.175514
1	4.621157	–3.314152	1.313048
6	2.955290	–2.713560	0.068824
1	2.340726	–3.577987	0.353589
6	3.691679	–3.102591	–1.227381

1	4.318251	–3.983831	–1.042450
1	2.956080	–3.429640	–1.974615
6	4.567874	–1.993817	–1.831340
1	5.520625	–1.963757	–1.300239
1	4.823651	–2.263208	–2.861952
6	3.928828	–0.593940	–1.828036
1	3.258563	–0.512456	–2.695292
1	4.713134	0.152645	–2.005229
6	1.211508	–1.635780	–1.466458
8	0.716556	–1.893434	–2.445315

3–BCI2

SCF energy = –1824.56972126

5	–2.720596	–0.073991	–0.398568
5	1.468443	–1.294917	–0.084435
15	0.263559	1.277518	0.163307
6	1.624406	2.440809	–0.075286
6	1.824735	2.975114	–1.350253
1	1.144015	2.726527	–2.158708
6	2.902472	3.816130	–1.583089
1	3.061402	4.227184	–2.573866
6	3.782691	4.120996	–0.549833
1	4.628820	4.773768	–0.736149
6	3.587019	3.584187	0.716738
1	4.280145	3.814673	1.518314
6	2.510222	2.740489	0.957664
1	2.370580	2.297521	1.938097
6	–1.289144	2.177767	–0.057881
6	–2.470547	1.486877	–0.404505
6	–3.596561	2.272366	–0.684497
1	–4.519195	1.787143	–0.984215
6	–3.580301	3.657648	–0.585151
1	–4.481402	4.223302	–0.798529
6	–2.410693	4.313671	–0.232672
1	–2.382910	5.395289	–0.158268
6	–1.262938	3.573530	0.008773
1	–0.339117	4.088687	0.248076
6	0.439899	0.369639	1.678297
6	1.002762	–0.905667	1.446424
6	1.123984	–1.699380	2.597289
1	1.547405	–2.691867	2.517693
6	0.711706	–1.262203	3.848389
1	0.821531	–1.922305	4.703655
6	0.154436	0.003128	4.026001
1	–0.171335	0.331174	5.007178
6	0.017389	0.829719	2.926108
1	–0.433092	1.813354	3.026164
6	–3.399160	–0.857111	–1.581474
1	–3.378195	–0.303573	–2.526583
6	–2.662108	–2.200259	–1.793767
1	–3.154160	–2.756930	–2.601011
1	–1.650301	–1.986479	–2.149677
6	–2.583966	–3.088904	–0.546297
1	–1.869816	–3.896643	–0.738449
1	–3.544512	–3.585438	–0.392393
6	–2.149161	–2.351456	0.731653
1	–1.059711	–2.279603	0.734036
1	–2.403707	–2.959018	1.609529
6	–2.693444	–0.922355	0.919193
1	–2.150316	–0.454036	1.744510
6	–4.209615	–0.869216	1.297701
1	–4.341410	–1.361658	2.267986
1	–4.500794	0.178524	1.454718
6	–5.144143	–1.510526	0.264345
1	–5.056798	–2.595330	0.332518
1	–6.181748	–1.284976	0.533828
6	–4.894650	–1.047459	–1.182772
1	–5.417754	–0.096690	–1.338679
1	–5.360888	–1.754202	–1.880057
6	3.035598	–0.819759	–0.348685
1	3.209992	0.219572	–0.042744
6	3.938018	–1.682419	0.552149
1	4.987873	–1.390418	0.410693
1	3.703082	–1.443668	1.596564
6	3.827771	–3.201672	0.345537
1	4.420333	–3.483867	–0.527381
1	4.308541	–3.708429	1.190887
6	2.394803	–3.744639	0.183163
1	1.968823	–3.942829	1.170963
1	2.452298	–4.730953	–0.297736
6	1.423032	–2.846252	–0.609826
1	0.423670	–3.285765	–0.486195
6	1.732902	–2.888451	–2.121702
1	1.732759	–3.931308	–2.468023
1	0.921036	–2.393141	–2.659859
6	3.068051	–2.242931	–2.531477
1	3.882991	–2.944847	–2.339526
1	3.070457	–2.093050	–3.617370
6	3.380040	–0.900986	–1.845881
1	2.829467	–0.105718	–2.365287
1	4.442956	–0.667675	–1.998579
6	0.542831	–0.309123	–0.999885
8	0.053293	–0.276543	–2.085956

3–BCI3

SCF energy = –1824.57726815

5	–2.059337	0.800694	–0.489609
5	2.096649	0.767371	–0.245587
15	0.184883	–1.367605	–0.245116
6	–0.303262	–2.158456	1.300463
6	–1.520893	–2.829276	1.404836
1	–2.202956	–2.856565	0.561722
6	–1.865081	–3.438306	2.603210
1	–2.813041	–3.957326	2.689186
6	–1.002495	–3.371513	3.691141
1	–1.277761	–3.842770	4.628518
6	0.213235	–2.704632	3.583405
1	0.886322	–2.655282	4.431951
6	0.570929	–2.101097	2.386853
1	1.525908	–1.593248	2.295283
6	–1.089583	–1.509707	–1.488106
6	–2.039683	–0.465065	–1.528971
6	–2.992508	–0.591271	–2.549771
1	–3.740766	0.180483	–2.668074
6	–3.007323	–1.658315	–3.437791
1	–3.769809	–1.698276	–4.209291
6	–2.046749	–2.661202	–3.365124
1	–2.049873	–3.485048	–4.070097
6	–1.071697	–2.578335	–2.388020
1	–0.293926	–3.333566	–2.331807
6	1.856874	–1.831650	–0.619953
6	2.732578	–0.727559	–0.535971
6	4.088823	–1.059193	–0.702557
1	4.843229	–0.286765	–0.640212
6	4.513606	–2.358046	–0.940426
1	5.574033	–2.553785	–1.066740
6	3.608304	–3.415824	–1.007285
1	3.953208	–4.428916	–1.182084
6	2.264549	–3.151602	–0.829070
1	1.541013	–3.961710	–0.835730
6	–2.593354	0.482050	1.005799
1	–2.169919	–0.432634	1.428787
6	–2.203386	1.614748	1.976712
1	–2.697801	1.459619	2.945186
1	–1.131763	1.513441	2.182874
6	–2.481025	3.054469	1.502883
1	–1.847885	3.739297	2.078555
1	–3.505900	3.330506	1.761518
6	–2.253915	3.312216	0.002295
1	–1.186363	3.462398	–0.176061
1	–2.737868	4.261101	–0.263350
6	–2.762459	2.190982	–0.931288
1	–2.489780	2.477153	–1.957238
6	–4.307128	2.090016	–0.885689
1	–4.737939	3.092902	–1.005322
1	–4.664067	1.529721	–1.755161
6	–4.904088	1.443449	0.376783
1	–4.984820	2.186460	1.172504
1	–5.934155	1.133897	0.166051
6	–4.111561	0.239968	0.900144
1	–4.282790	–0.619262	0.236560
1	–4.513712	–0.051118	1.879459
6	2.474219	1.407879	1.240821
1	2.211216	0.720786	2.058739
6	3.999800	1.597319	1.304548
1	4.264948	2.077611	2.256261
1	4.465312	0.607153	1.343448
6	4.622759	2.422513	0.160736
1	4.540977	3.481846	0.411652
1	5.700741	2.223190	0.129555
6	4.031540	2.199188	–1.248400
1	4.538364	1.362102	–1.736296
1	4.280918	3.074428	–1.863316
6	2.512318	1.950991	–1.310515
1	2.287437	1.635714	–2.338708
6	1.710953	3.238117	–1.048586
1	2.041699	4.022672	–1.742500
1	0.660865	3.054094	–1.288638
6	1.810946	3.778756	0.385490
1	2.753673	4.317432	0.506845
1	1.028159	4.530759	0.538993
6	1.687323	2.709368	1.482780
1	0.627893	2.464025	1.605939
1	1.998101	3.150392	2.439511
6	0.522488	0.478350	–0.238687
8	–0.455157	1.218108	–0.347734

3–BCl4

SCF energy = –1824.58960326

5	2.016690	–0.557226	–0.540840
5	–0.261403	1.735063	0.642658
15	–1.011968	–0.827062	0.122392
6	–2.748063	–1.181560	–0.254541
6	–3.075405	–1.607684	–1.544743
1	–2.292023	–1.794130	–2.271998

6	–4.402828	–1.810491	–1.892093
1	–4.651086	–2.140183	–2.894922
6	–5.409257	–1.594789	–0.956741
1	–6.446671	–1.755824	–1.229609
6	–5.087041	–1.177708	0.328369
1	–5.869485	–1.012954	1.061042
6	–3.760102	–0.966268	0.680280
1	–3.516407	–0.625752	1.680642
6	–0.037618	–2.249843	–0.338932
6	1.316327	–2.037406	–0.674886
6	1.994195	–3.197836	–1.083550
1	3.028428	–3.116221	–1.386319
6	1.404001	–4.451287	–1.112451
1	1.987794	–5.310475	–1.429797
6	0.072975	–4.620862	–0.740706
1	–0.390653	–5.601321	–0.757182
6	–0.655078	–3.509619	–0.363746
1	–1.702368	–3.618663	–0.099538
6	–0.903222	–0.348232	1.857422
6	–0.558318	1.005667	1.995116
6	–0.437805	1.521508	3.287331
1	–0.162541	2.562166	3.428444
6	–0.636510	0.704762	4.391501
1	–0.524241	1.109323	5.391911
6	–0.961034	–0.641455	4.225808
1	–1.096570	–1.274230	5.096476
6	–1.100363	–1.179465	2.953522
1	–1.336978	–2.230454	2.820980
6	3.358841	–0.264150	–1.433384
1	3.173906	–0.486588	–2.495052
6	3.650830	1.246757	–1.340507
1	4.536599	1.501942	–1.939944
1	2.811565	1.783727	–1.790006
6	3.879008	1.753394	0.094032
1	3.834227	2.849948	0.103730
1	4.901176	1.514832	0.397487
6	2.898023	1.206355	1.149160
1	1.984456	1.816557	1.106216
1	3.309987	1.397714	2.151042
6	2.488635	–0.269896	1.004390
1	1.692767	–0.446927	1.740552
6	3.607595	–1.259457	1.377691
1	3.902098	–1.121029	2.427826
1	3.195288	–2.274843	1.316728
6	4.867351	–1.175465	0.505866
1	5.461776	–0.317827	0.830512
1	5.498973	–2.049688	0.705049
6	4.603403	–1.077817	–1.009866
1	4.536144	–2.090385	–1.417756
1	5.496427	–0.651289	–1.488876
6	–1.153915	1.347894	–1.752880
1	–1.438879	0.514239	–2.408204
6	–2.476851	1.962964	–1.231848
1	–3.225004	1.854164	–2.024394
1	–2.866521	1.357104	–0.406317
6	–2.501343	3.432140	–0.789666
1	–2.291821	4.067035	–1.649822
1	–3.536645	3.663655	–0.513492
6	–1.611141	3.831837	0.399549
1	–2.113009	3.524417	1.326100
1	–1.565177	4.926961	0.439715
6	–0.156990	3.282452	0.439860
1	0.280064	3.709462	1.354024
6	0.746521	3.738032	–0.723010
1	0.994945	4.795643	–0.567139
1	1.690727	3.196074	–0.650156
6	0.214928	3.617943	–2.156857
1	–0.541190	4.389627	–2.315031
1	1.038556	3.901921	–2.821676
6	–0.304865	2.257769	–2.662123
1	0.547692	1.649379	–2.966763
1	–0.889937	2.446790	–3.570662
6	–0.278646	0.750839	–0.617424
8	0.984908	0.458586	–1.086059

CO

SCF energy = –113.305480104

6	0.000000	0.000000	–0.642927
8	0.000000	0.000000	0.482195

3–CyI1

SCF energy = –2025.68039318

5	–1.723986	0.370782	1.105548
5	2.280132	–0.089527	–0.150059
15	–1.245897	0.776670	–0.809164
6	–2.591107	0.118363	–1.848505
6	–2.451879	–1.141652	–2.433455
1	–1.515821	–1.680630	–2.354709
6	–3.514296	–1.709139	–3.121804
1	–3.397429	–2.688855	–3.571878
6	–4.719698	–1.025486	–3.234655
1	–5.549887	–1.472729	–3.770762

6	–4.859200	0.231587	–2.660894
1	–5.796668	0.769882	–2.749049
6	–3.800336	0.802804	–1.965403
1	–3.924515	1.775872	–1.502498
6	–1.789222	2.357080	–0.126040
6	–2.094244	1.916619	1.165969
6	–2.614665	2.825780	2.087116
1	–2.868546	2.519677	3.097194
6	–2.776004	4.147436	1.694110
1	–3.161754	4.874707	2.401136
6	–2.437263	4.570465	0.402609
1	–2.564756	5.614619	0.137113
6	–1.941300	3.675225	–0.535323
1	–1.671382	3.995432	–1.536021
6	0.249381	0.975218	–1.820814
6	1.605350	0.742441	–1.468768
6	2.491946	1.208956	–2.466419
1	3.552324	1.095210	–2.307589
6	2.122156	1.810832	–3.657307
1	2.891211	2.128012	–4.355418
6	0.782483	2.001271	–3.959219
1	0.465554	2.460224	–4.889445
6	–0.146361	1.580896	–3.031438
1	–1.199907	1.717627	–3.258698
6	1.765345	0.446403	1.347732
6	0.511552	–0.043150	2.060703
6	0.424289	0.358099	3.528813
6	0.604135	1.864689	3.725355
6	1.845094	2.389396	3.002296
6	1.859566	1.969967	1.530479
1	2.528095	0.006239	2.005344
1	0.327727	–1.103972	1.921301
1	–0.352449	0.515198	1.553258
1	–0.518919	0.018413	3.971395
1	1.221631	–0.183639	4.052404
1	0.652779	2.095168	4.794700
1	–0.277552	2.385990	3.335492
1	1.895264	3.479612	3.098704
1	2.744321	1.991355	3.490577
1	2.762744	2.347963	1.044897
1	1.023185	2.454953	1.005127
6	–2.551925	–0.812178	1.739094
6	–2.190828	–2.251677	1.346551
6	–3.091803	–3.282668	2.026350
6	–4.568615	–3.014936	1.742774
6	–4.948059	–1.591073	2.144854
6	–4.054730	–0.560936	1.454854
1	–2.422752	–0.719045	2.830921
1	–1.150203	–2.471753	1.591057
1	–2.279690	–2.363197	0.258362
1	–2.813996	–4.288717	1.696142
1	–2.920027	–3.251436	3.110543
1	–5.197209	–3.740797	2.268236
1	–4.760840	–3.149773	0.670178
1	–5.997554	–1.392461	1.903906
1	–4.850174	–1.482432	3.233169
1	–4.340481	0.448556	1.765958
1	–4.228729	–0.611577	0.373076
6	2.020549	–1.720725	–0.402157
1	2.676290	–2.010575	–1.236034
6	0.618074	–2.116987	–0.876589
1	0.431831	–1.614951	–1.830085
1	–0.139584	–1.747031	–0.177172
6	0.406223	–3.620507	–1.073702
1	–0.645519	–3.830573	–1.311776
1	0.992990	–3.948572	–1.941932
6	0.842043	–4.432000	0.144566
1	0.725968	–5.503877	–0.050333
1	0.186786	–4.200288	0.995654
6	2.285381	–4.100991	0.518142
1	2.947678	–4.401301	–0.305038
1	2.593821	–4.681791	1.395271
6	2.456978	–2.603669	0.781533
1	3.502069	–2.397840	1.027243
1	1.891140	–2.354079	1.689050
6	3.962968	0.207308	–0.155108
1	4.101446	1.240713	–0.512345
6	4.766100	–0.696982	–1.117329
1	4.274743	–0.792402	–2.090425
1	4.789713	–1.716459	–0.709402
6	6.210156	–0.236182	–1.319757
1	6.730549	–0.899547	–2.020787
1	6.212899	0.764285	–1.775290
6	6.956110	–0.186690	0.011659
1	7.971560	0.202623	–0.124284
1	7.062115	–1.209117	0.399076
6	6.191259	0.657154	1.028145
1	6.200494	1.705913	0.699907
1	6.699823	0.632271	1.999309
6	4.733267	0.209326	1.185814
1	4.268424	0.882835	1.911049
1	4.715659	–0.788388	1.645251

3–CyI2

SCF energy = –2025.75751194

5	2.095445	–0.074365	–0.143450
5	–2.036437	0.590818	0.142242
15	–0.957867	–1.033808	–0.223556
6	–2.152310	–2.369824	–0.537353
6	–3.516194	–2.129763	–0.691716
1	–3.919084	–1.127328	–0.594733
6	–4.380793	–3.178847	–0.982608
1	–5.441269	–2.986060	–1.101615
6	–3.884387	–4.467561	–1.123862
1	–4.559473	–5.285228	–1.352752
6	–2.522375	–4.711025	–0.975864
1	–2.132141	–5.716316	–1.090123
6	–1.656995	–3.667747	–0.685658
1	–0.594709	–3.856145	–0.569781
6	0.001089	–0.809463	–1.721738
6	1.330330	–0.369899	–1.599072
6	1.953716	–0.129694	–2.840012
1	2.978333	0.219661	–2.856491
6	1.326829	–0.307389	–4.062208
1	1.871208	–0.094790	–4.977589
6	0.014640	–0.766005	–4.128434
1	–0.474619	–0.928252	–5.082808
6	–0.649907	–1.019527	–2.945600
1	–1.666769	–1.399875	–2.971889
6	0.161030	–1.549772	1.072107
6	1.474022	–1.049738	1.039661
6	2.236065	–1.393939	2.172927
1	3.253452	–1.034817	2.239425
6	1.749585	–2.160488	3.217929
1	2.393892	–2.383914	4.063130
6	0.446903	–2.654947	3.190347
1	0.065799	–3.270614	3.998054
6	–0.351469	–2.342209	2.109373
1	–1.371102	–2.714248	2.067423
6	–2.577251	1.279890	–1.156573
6	–1.511968	2.344447	–1.555268
6	–1.918129	3.067022	–2.839672
6	–3.307467	3.692698	–2.727761
6	–4.355223	2.652849	–2.329903
6	–3.962014	1.937118	–1.037063
1	–2.612274	0.571773	–1.995793
1	–0.533933	1.879673	–1.696113
1	–1.400253	3.072605	–0.741575
1	–1.170858	3.831128	–3.074821
1	–1.901591	2.346315	–3.666725
1	–3.585827	4.169941	–3.672451
1	–3.285094	4.487806	–1.971105
1	–5.335310	3.125973	–2.211761
1	–4.458865	1.913673	–3.135060
1	–4.721447	1.188726	–0.781073
1	–3.959951	2.664527	–0.216879
6	1.705224	1.501469	0.263827
6	2.232737	2.522241	–0.758025
6	1.874461	3.971863	–0.427411
6	2.333312	4.349864	0.978974
6	1.740122	3.389145	2.006914
6	2.094640	1.932865	1.689897
1	0.597745	1.583481	0.229945
1	1.863271	2.278380	–1.759393
1	3.326005	2.438237	–0.817360
1	2.313076	4.649954	–1.168662
1	0.784984	4.101518	–0.495149
1	2.057193	5.384313	1.212095
1	3.429530	4.299680	1.026456
1	2.079937	3.647903	3.016390
1	0.648484	3.518481	2.007195
1	1.624580	1.272216	2.424339
1	3.170906	1.807404	1.837707
6	3.723092	–0.346612	–0.397115
6	4.013588	–1.840142	–0.641022
6	5.431805	–2.107325	–1.147172
6	6.474612	–1.514567	–0.200902
6	6.220844	–0.024283	0.018931
6	4.802365	0.244063	0.533691
1	3.952624	0.153282	–1.348106
1	3.286405	–2.247797	–1.352843
1	3.863866	–2.400043	0.291766
1	5.599379	–3.183515	–1.273174
1	5.551806	–1.654363	–2.141257
1	7.486433	–1.678610	–0.588511
1	6.421063	–2.035493	0.765116
1	6.959912	0.388790	0.715468
1	6.360975	0.504862	–0.933877
1	4.669323	1.324811	0.626673
1	4.733168	–0.154715	1.552925
6	–2.395457	1.037464	1.597401
6	–1.253469	1.160486	2.619548
6	–1.773678	1.577924	3.992945
6	–2.828319	0.597996	4.504907
6	–3.978359	0.461863	3.507687
6	–3.480078	0.052266	2.120084

1	–2.881227	2.021595	1.535365
1	–0.525669	1.887605	2.262378
1	–0.717721	0.212970	2.714592
1	–0.938943	1.641753	4.697517
1	–2.209888	2.583883	3.931348
1	–3.212082	0.917710	5.478784
1	–2.361375	–0.383951	4.656566
1	–4.710644	–0.270363	3.863353
1	–4.505522	1.421038	3.427591
1	–4.330115	0.004265	1.430353
1	–3.063636	–0.961250	2.176085

3–CyPB

SCF energy = –1295.12681682

5	–1.413730	0.205122	–0.092501
15	1.571986	–0.032307	–1.232094
6	0.634328	–1.365183	–0.394882
6	1.253003	–2.612904	–0.274008
1	2.278838	–2.744146	–0.605573
6	0.582207	–3.681424	0.296356
1	1.083481	–4.637886	0.405406
6	–0.730047	–3.523689	0.731081
1	–1.260762	–4.355858	1.181766
6	–1.357250	–2.300235	0.573394
1	–2.381895	–2.200446	0.910961
6	–0.703745	–1.187534	0.013113
6	3.191062	–0.130572	–0.363280
6	3.291598	–0.121205	1.031278
6	4.531398	–0.196366	1.645751
1	4.600031	–0.189340	2.728729
6	5.689137	–0.280197	0.875027
1	6.658930	–0.339972	1.358192
6	5.600791	–0.289184	–0.509293
1	6.500226	–0.354357	–1.112738
6	4.354174	–0.214584	–1.125762
1	4.284146	–0.223246	–2.209355
6	0.841250	1.458861	–0.463432
6	–0.512766	1.485613	–0.077487
6	–1.030242	2.707091	0.388745
1	–2.072239	2.764901	0.688422
6	–0.247116	3.843764	0.493752
1	–0.671822	4.766737	0.874696
6	1.085981	3.796464	0.096328
1	1.708587	4.682816	0.166302
6	1.620581	2.616804	–0.395121
1	2.660562	2.590553	–0.707221
6	–2.993118	0.372447	–0.183613
1	–3.188698	1.381558	–0.575192
6	–3.682240	0.322599	1.201730
1	–3.226028	1.050770	1.881611
1	–3.529477	–0.656835	1.669976
6	–5.185840	0.584997	1.091156
1	–5.653980	0.506089	2.078099
1	–5.347060	1.615667	0.748926
6	–5.850310	–0.381312	0.109699
1	–6.919531	–0.161716	0.025264
1	–5.772558	–1.403446	0.504463
6	–5.184304	–0.321982	–1.265130
1	–5.345276	0.672355	–1.702229
1	–5.653426	–1.040502	–1.945416
6	–3.682414	–0.593933	–1.168001
1	–3.222490	–0.504987	–2.158251
1	–3.527218	–1.633093	–0.859378
1	2.389796	–0.056644	1.632053

3–CyTS1

SCF energy = –2025.68001784

5	–1.853400	0.095018	–0.008202
5	1.904989	0.633260	–0.122500
15	1.047317	–1.005246	0.569956
6	1.424207	–2.746580	0.283059
6	2.730696	–3.177096	0.043410
1	3.549624	–2.468363	0.033439
6	2.984297	–4.524869	–0.170409
1	4.000203	–4.858126	–0.351681
6	1.941084	–5.442671	–0.144222
1	2.142733	–6.495576	–0.310516
6	0.639956	–5.017171	0.101185
1	–0.173262	–5.734019	0.126519
6	0.377652	–3.672429	0.315630
1	–0.635359	–3.338834	0.513169
6	–0.220043	–0.832167	1.821908
6	–1.397704	–0.142442	1.541680
6	–2.188199	0.150231	2.666405
1	–3.133937	0.662317	2.530979
6	–1.823151	–0.218208	3.950379
1	–2.470106	0.033618	4.785215
6	–0.641809	–0.922033	4.181044
1	–0.362941	–1.224005	5.184716
6	0.174944	–1.223779	3.108465
1	1.109975	–1.754575	3.270625
6	–0.624758	–0.492822	–1.009363

6	0.779226	–0.095047	–1.184046
6	1.469096	–0.596593	–2.355383
1	2.471755	–0.248231	–2.546750
6	0.902347	–1.420673	–3.273779
1	1.448515	–1.706763	–4.166335
6	–0.396939	–1.902170	–3.037892
1	–0.851543	–2.610944	–3.722984
6	–1.098021	–1.452136	–1.957750
1	–2.099608	–1.819658	–1.829659
6	3.470743	0.311799	–0.465296
6	4.304063	0.142071	0.821991
6	5.758761	–0.225208	0.522807
6	6.416847	0.802227	–0.397765
6	5.602920	0.999661	–1.675641
6	4.152407	1.367831	–1.357690
1	3.574693	–0.643920	–0.996797
1	3.855080	–0.621874	1.468707
1	4.285973	1.069749	1.406159
1	6.323879	–0.317607	1.456182
1	5.793090	–1.212307	0.039698
1	7.441444	0.499857	–0.637702
1	6.491345	1.761494	0.130905
1	6.060760	1.772889	–2.301283
1	5.620239	0.071409	–2.263531
1	3.597404	1.517329	–2.290797
1	4.138855	2.338289	–0.847094
6	–2.049279	1.693464	–0.427615
6	–3.271625	2.375479	0.213867
6	–3.399588	3.856438	–0.149626
6	–3.412154	4.061236	–1.662113
6	–2.157674	3.459290	–2.289842
6	–2.010364	1.974822	–1.944331
1	–1.184789	2.221345	–0.014902
1	–3.212026	2.290228	1.302954
1	–4.198315	1.868809	–0.081208
1	–4.304887	4.278094	0.301912
1	–2.553007	4.410083	0.276801
1	–3.491944	5.126479	–1.905441
1	–4.301200	3.575371	–2.087174
1	–2.171060	3.593479	–3.377589
1	–1.281021	4.008819	–1.920603
1	–1.067431	1.609684	–2.368325
1	–2.798726	1.414932	–2.460323
6	–3.306554	–0.756563	–0.081688
6	–3.269354	–2.225025	0.399191
6	–4.662447	–2.810285	0.642376
6	–5.544629	–2.682275	–0.597445
6	–5.623293	–1.227872	–1.056575
6	–4.233602	–0.634914	–1.311200
1	–3.874246	–0.239566	0.707786
1	–2.687038	–2.301313	1.323053
1	–2.760933	–2.870192	–0.331622
1	–4.586038	–3.859934	0.950004
1	–5.133606	–2.274471	1.477155
1	–6.546464	–3.079697	–0.401431
1	–5.120307	–3.293759	–1.406454
1	–6.239818	–1.146119	–1.959037
1	–6.126980	–0.635318	–0.280746
1	–4.348684	0.413673	–1.590519
1	–3.813238	–1.124989	–2.198831
6	1.703656	2.071221	0.585655
6	0.852670	2.263224	1.848400
6	0.957033	3.695226	2.373456
6	0.551706	4.706952	1.302035
6	1.397117	4.543523	0.039094
6	1.345129	3.111900	–0.496627
1	2.720735	2.336939	0.910424
1	1.170478	1.557891	2.623885
1	–0.197383	2.042554	1.656045
1	0.329367	3.812514	3.263096
1	1.990220	3.896912	2.689172
1	0.638325	5.728528	1.687347
1	–0.505281	4.555055	1.051016
1	1.064486	5.244550	–0.734501
1	2.439665	4.803779	0.269062
1	2.022855	3.021507	–1.351335
1	0.349556	2.905874	–0.891119

3–CyTS2

SCF energy = –2025.70864331

5	1.023582	–0.932437	–0.293639
5	–1.819927	0.287653	0.108952
15	1.275028	0.952265	0.359452
6	2.756473	1.949319	0.638180
6	3.911703	1.383937	1.175722
1	3.939643	0.326103	1.413529
6	5.024063	2.179360	1.421408
1	5.920657	1.736433	1.840766
6	4.985927	3.537583	1.130986
1	5.856566	4.156052	1.321300
6	3.831663	4.107641	0.604625
1	3.797240	5.170161	0.389837
6	2.716288	3.318181	0.362329

1	1.806981	3.768756	–0.023758
6	0.442023	1.290188	–1.191124
6	–0.417301	0.155958	–1.176282
6	–0.878924	–0.259262	–2.438927
1	–1.522698	–1.128908	–2.506815
6	–0.516123	0.406513	–3.604257
1	–0.868126	0.047459	–4.565634
6	0.297773	1.532036	–3.546260
1	0.570509	2.045044	–4.463031
6	0.804615	1.984387	–2.325945
1	1.511973	2.806393	–2.293710
6	0.130066	1.211349	1.723922
6	–1.171678	0.714451	1.546360
6	–2.007553	0.847079	2.666238
1	–3.043113	0.539840	2.588327
6	–1.578707	1.397969	3.864742
1	–2.271514	1.471375	4.697576
6	–0.278610	1.870345	3.999885
1	0.060216	2.309694	4.931903
6	0.579634	1.779446	2.917110
1	1.595776	2.152211	3.002097
6	–2.589152	–1.184798	0.035406
6	–3.775664	–1.285405	–0.945516
6	–4.343601	–2.701299	–1.074566
6	–4.759211	–3.277070	0.274967
6	–3.592214	–3.202242	1.254157
6	–3.064863	–1.771707	1.381175
1	–1.837192	–1.899230	–0.329490
1	–3.494327	–0.951774	–1.944835
1	–4.574911	–0.604311	–0.622490
1	–5.190497	–2.702132	–1.770122
1	–3.576981	–3.352828	–1.517565
1	–5.108860	–4.309259	0.164070
1	–5.604893	–2.699700	0.671899
1	–3.889222	–3.583142	2.238077
1	–2.786585	–3.856333	0.896737
1	–2.264438	–1.745637	2.125635
1	–3.877201	–1.153059	1.786594
6	2.024520	–1.319058	–1.500559
6	1.531454	–2.422673	–2.457211
6	2.483045	–2.595857	–3.642012
6	3.896606	–2.937252	–3.169989
6	4.409306	–1.909512	–2.161351
6	3.428248	–1.719978	–1.001780
1	2.169174	–0.427098	–2.128538
1	0.528327	–2.200746	–2.825649
1	1.457647	–3.376413	–1.925313
1	2.112540	–3.375687	–4.316204
1	2.506062	–1.663773	–4.222940
1	4.580961	–3.007728	–4.022061
1	3.884549	–3.928115	–2.696950
1	5.390990	–2.210687	–1.779542
1	4.552156	–0.944918	–2.666250
1	3.826479	–0.968424	–0.313918
1	3.362171	–2.655871	–0.432867
6	0.647236	–1.919247	0.915072
6	1.715483	–1.852287	2.030896
6	1.315698	–2.676252	3.255086
6	1.040124	–4.131700	2.881590
6	–0.005301	–4.219208	1.771243
6	0.406465	–3.393826	0.550046
1	–0.276298	–1.557900	1.375615
1	1.877413	–0.816427	2.350525
1	2.679042	–2.215988	1.651601
1	2.098043	–2.620026	4.019982
1	0.412716	–2.234171	3.695688
1	0.711808	–4.695430	3.761092
1	1.973160	–4.600245	2.539805
1	–0.170737	–5.263433	1.484514
1	–0.961489	–3.844515	2.154583
1	–0.354577	–3.479100	–0.232302
1	1.324618	–3.827369	0.134145
6	–2.716656	1.624847	–0.343849
6	–3.093313	1.809584	–1.824255
6	–4.151113	2.894169	–2.041001
6	–3.660712	4.243275	–1.522144
6	–3.216192	4.126198	–0.067355
6	–2.203331	2.997191	0.146415
1	–3.661664	1.443656	0.202616
1	–3.437502	0.883090	–2.279973
1	–2.194348	2.105447	–2.376312
1	–4.403338	2.966317	–3.105297
1	–5.074863	2.612849	–1.517982
1	–4.437339	5.008817	–1.628652
1	–2.809761	4.571591	–2.134830
1	–2.794955	5.076556	0.280790
1	–4.095359	3.929542	0.561200
1	–1.943640	2.976558	1.205140
1	–1.273863	3.242141	–0.390032

3–CyTS3

SCF energy = –2025.69969737

5	1.972242	–0.494628	–0.090649
5	–1.071444	0.881357	0.075498
15	–0.900764	–1.127717	–0.104355
6	–2.423518	–2.114246	–0.218980
6	–3.663118	–1.510946	–0.417765
1	–3.740758	–0.433269	–0.478737
6	–4.809030	–2.287277	–0.551447
1	–5.768833	–1.805824	–0.703448
6	–4.722253	–3.671100	–0.492039
1	–5.617054	–4.276003	–0.593899
6	–3.485705	–4.282519	–0.309082
1	–3.411610	–5.364019	–0.271448
6	–2.341277	–3.510531	–0.177651
1	–1.377800	–3.991936	–0.046670
6	0.069467	–1.515478	–1.565252
6	1.375364	–1.016563	–1.500083
6	2.112670	–1.101551	–2.690863
1	3.124833	–0.716608	–2.732360
6	1.598468	–1.689253	–3.837604
1	2.206545	–1.735028	–4.735772
6	0.320447	–2.237337	–3.837527
1	–0.073529	–2.721306	–4.724908
6	–0.454055	–2.140096	–2.694383
1	–1.467780	–2.527720	–2.690607
6	0.112172	–1.777479	1.230608
6	1.428633	–1.292296	1.195502
6	2.211836	–1.587442	2.319400
1	3.225439	–1.214267	2.377614
6	1.733384	–2.350782	3.375088
1	2.377308	–2.556615	4.224447
6	0.439666	–2.859442	3.346479
1	0.067606	–3.468196	4.163759
6	–0.381067	–2.557771	2.272762
1	–1.409575	–2.902594	2.265124
6	–1.833533	1.529178	–1.225842
6	–1.632621	0.952988	–2.635852
6	–2.567512	1.597598	–3.663804
6	–2.470029	3.120741	–3.682274
6	–2.686500	3.692651	–2.282463
6	–1.704302	3.064438	–1.295411
1	–2.895479	1.341667	–1.009523
1	–1.841007	–0.116545	–2.639824
1	–0.589154	1.053886	–2.958106
1	–2.360657	1.188803	–4.658628
1	–3.601686	1.313809	–3.422349
1	–3.193419	3.540600	–4.389281
1	–1.474830	3.417292	–4.039333
1	–2.567087	4.781393	–2.292354
1	–3.716275	3.491411	–1.957200
1	–1.819332	3.522018	–0.306648
1	–0.695733	3.315893	–1.632485
6	0.858706	1.449397	0.187158
6	1.623853	2.187084	–0.944337
6	1.791370	3.691167	–0.679668
6	2.375347	3.975289	0.703480
6	1.532621	3.324192	1.800018
6	1.379958	1.813671	1.591981
1	–0.041708	2.106561	0.156143
1	1.109570	2.021871	–1.894984
1	2.619491	1.770439	–1.083142
1	2.427192	4.128807	–1.457599
1	0.823974	4.200774	–0.749356
1	2.438415	5.056459	0.866755
1	3.403948	3.599405	0.757785
1	1.971746	3.521311	2.784431
1	0.537696	3.792716	1.805135
1	0.712498	1.412945	2.353339
1	2.335076	1.331315	1.785858
6	3.583231	–0.243175	–0.202769
6	4.248999	–1.645751	–0.288447
6	5.702606	–1.562906	–0.753901
6	6.525489	–0.666506	0.168991
6	5.884640	0.713458	0.299756
6	4.420029	0.637772	0.742869
1	3.758540	0.207357	–1.188433
1	3.686534	–2.305490	–0.954097
1	4.224674	–2.130376	0.693218
1	6.140828	–2.565780	–0.801306
1	5.734995	–1.159313	–1.775238
1	7.553951	–0.576228	–0.196582
1	6.586683	–1.133488	1.161227
1	6.454421	1.332622	1.001168
1	5.932906	1.223259	–0.672197
1	4.022767	1.651990	0.768959
1	4.382654	0.272954	1.776031
6	–1.777001	1.344062	1.507914
6	–1.629763	0.392822	2.710058
6	–2.121357	1.006095	4.020038
6	–3.581260	1.438100	3.920456
6	–3.786621	2.359500	2.721190
6	–3.270643	1.734339	1.422405

1	–1.265615	2.275013	1.798535
1	–0.600138	0.061498	2.838783
1	–2.212841	–0.518634	2.515709
1	–1.988398	0.289673	4.837898
1	–1.497650	1.877099	4.263530
1	–3.905585	1.929710	4.843645
1	–4.211856	0.546654	3.801830
1	–4.846705	2.614162	2.613147
1	–3.255998	3.305233	2.895439
1	–3.457471	2.437656	0.608811
1	–3.874008	0.842547	1.207020

BCy3

SCF energy = –730.624138729

5	0.142202	–0.047791	–0.238213
6	1.705561	–0.122205	0.114978
6	2.564952	0.922458	–0.629407
6	4.033287	0.904705	–0.203055
6	4.644057	–0.487454	–0.341769
6	3.829839	–1.512063	0.444401
6	2.359751	–1.511845	0.021727
1	1.737258	0.159156	1.185191
1	2.162930	1.927764	–0.477634
1	2.505783	0.731142	–1.710375
1	4.602229	1.632168	–0.791911
1	4.105274	1.225937	0.844865
1	5.685573	–0.484158	–0.003889
1	4.660018	–0.772136	–1.402438
1	4.255239	–2.513680	0.320475
1	3.896019	–1.276606	1.515358
1	1.813864	–2.228482	0.643249
1	2.285025	–1.883289	–1.009983
6	–0.489068	1.413022	–0.349562
6	–0.327292	2.136989	1.013470
6	–0.769393	3.599770	0.954542
6	–2.199407	3.739528	0.436978
6	–2.360227	3.044675	–0.913458
6	–1.935035	1.576605	–0.842556
1	0.143741	1.967630	–1.061467
1	0.709727	2.089738	1.357221
1	–0.925216	1.611686	1.771394
1	–0.674379	4.059352	1.944224
1	–0.090182	4.148413	0.288506
1	–2.474322	4.796525	0.359367
1	–2.892113	3.288684	1.160178
1	–3.396639	3.120257	–1.259222
1	–1.744174	3.562307	–1.661113
1	–2.053587	1.117164	–1.827834
1	–2.618819	1.046118	–0.167297
6	–0.688560	–1.399984	–0.249876
1	0.008925	–2.235660	–0.388311
6	–1.814840	–1.634209	–1.270693
1	–1.428435	–1.533067	–2.291027
1	–2.601150	–0.883731	–1.161998
6	–2.443324	–3.016456	–1.081580
1	–3.240313	–3.173210	–1.816139
1	–1.688401	–3.791708	–1.268365
6	–2.994526	–3.176050	0.336294
1	–3.422929	–4.174479	0.471934
1	–3.816174	–2.462129	0.482390
6	–1.915210	–2.917555	1.388526
1	–1.148522	–3.700051	1.321393
1	–2.343295	–2.983828	2.394553
6	–1.248679	–1.553913	1.189901
1	–0.452367	–1.424481	1.933144
1	–1.982914	–0.760505	1.383461

3–Cy

SCF energy = –2025.77544991

5	–2.599935	–0.929624	0.028951
5	1.890834	1.615221	–0.238466
15	0.447684	–1.192071	–0.315816
6	1.958923	–2.178757	0.040371
6	2.093089	–2.708400	1.324742
1	1.309644	–2.541635	2.058979
6	3.224336	–3.433334	1.677885
1	3.316987	–3.836559	2.680926
6	4.242971	–3.626369	0.752056
1	5.133310	–4.180840	1.029977
6	4.120563	–3.099676	–0.528412
1	4.913971	–3.243505	–1.254742
6	2.984608	–2.382652	–0.883407
1	2.904293	–1.956904	–1.878245
6	–0.717276	–2.455942	–0.963664
6	–2.082676	–2.150943	–0.838516
6	–3.008030	–3.024838	–1.420761
1	–4.071135	–2.805787	–1.356492
6	–2.599037	–4.188714	–2.059498
1	–3.337594	–4.859710	–2.486925
6	–1.246821	–4.499156	–2.140332
1	–0.922069	–5.412737	–2.627505
6	–0.309616	–3.628543	–1.601014

1	0.747878	–3.861892	–1.676382
6	0.929991	–0.253304	–1.833482
6	1.511624	1.017405	–1.651710
6	1.840599	1.758604	–2.791627
1	2.287959	2.742469	–2.680799
6	1.603562	1.273112	–4.071939
1	1.868156	1.872860	–4.937095
6	1.011814	0.029651	–4.236867
1	0.806828	–0.354707	–5.230732
6	0.674307	–0.724880	–3.120039
1	0.193078	–1.686918	–3.257668
6	3.148424	1.001704	0.495175
6	3.047158	0.810971	2.015057
6	4.347610	0.248061	2.588937
6	5.542810	1.136064	2.240497
6	5.650193	1.360598	0.731753
6	4.347746	1.922049	0.155556
1	3.391617	0.026742	0.059721
1	2.219942	0.133492	2.251888
1	2.816792	1.768763	2.500826
1	4.263960	0.132895	3.674989
1	4.506275	–0.757022	2.177191
1	6.469086	0.695908	2.624294
1	5.428730	2.107274	2.740698
1	6.482278	2.036112	0.505571
1	5.873115	0.406094	0.238349
1	4.447859	2.040579	–0.930074
1	4.174018	2.925544	0.567071
6	–2.698003	–1.225980	1.583893
6	–4.163941	–1.649542	1.861420
6	–4.363121	–2.076104	3.317414
6	–3.902519	–0.989826	4.289578
6	–2.451360	–0.589726	4.024112
6	–2.252568	–0.141840	2.575681
1	–2.083007	–2.114519	1.791552
1	–4.455903	–2.471800	1.197612
1	–4.840590	–0.814832	1.638851
1	–5.416029	–2.321711	3.492787
1	–3.791347	–2.994505	3.502079
1	–4.024289	–1.330975	5.322855
1	–4.545678	–0.106953	4.174754
1	–2.145696	0.207840	4.709728
1	–1.796817	–1.446886	4.231918
1	–1.200628	0.094497	2.400538
1	–2.811647	0.784488	2.412376
6	–3.228028	0.294569	–0.754459
6	–2.361788	0.742568	–1.950256
6	–3.061788	1.768891	–2.837429
6	–3.516132	2.981426	–2.028289
6	–4.402454	2.557421	–0.857188
6	–3.719656	1.516628	0.033852
1	–4.124670	–0.188954	–1.198371
1	–2.062893	–0.122323	–2.547421
1	–1.430427	1.183983	–1.574491
1	–2.389274	2.078105	–3.644452
1	–3.934397	1.301653	–3.313775
1	–4.047901	3.694096	–2.667192
1	–2.631057	3.506424	–1.646304
1	–4.685105	3.430905	–0.259175
1	–5.336734	2.135381	–1.251800
1	–4.408099	1.213644	0.828320
1	–2.866042	1.985067	0.533727
6	1.128248	2.854386	0.377754
6	–0.002852	2.290208	1.271911
6	–0.752982	3.400384	2.008202
6	–1.298192	4.456369	1.047026
6	–0.205767	4.998978	0.125634
6	0.532741	3.874778	–0.603539
1	1.815370	3.392097	1.049886
1	0.397096	1.575382	1.995142
1	–0.704133	1.723077	0.648597
1	–1.569134	2.965853	2.596162
1	–0.070092	3.876194	2.723898
1	–1.762576	5.274530	1.607376
1	–2.092805	4.013086	0.436618
1	–0.637505	5.698054	–0.598713
1	0.516258	5.573908	0.720646
1	1.317734	4.308092	–1.232955
1	–0.156980	3.361867	–1.286247

3–Cy–H

SCF energy = –2026.93372436

5	–2.273044	–0.829805	0.109255
5	1.803770	1.758607	–0.314903
15	0.712946	–1.367002	–0.217903
6	2.341606	–2.138533	0.015272
6	2.685075	–2.564106	1.298559
1	1.981909	–2.451900	2.119090
6	3.930635	–3.129467	1.533391
1	4.195575	–3.452739	2.533967
6	4.837603	–3.268131	0.489068
1	5.813925	–3.702822	0.674167
6	4.496203	–2.849133	–0.791801

1	5.205413	–2.954239	–1.605438
6	3.249837	–2.285502	–1.031530
1	2.993658	–1.938999	–2.027369
6	–0.494449	–2.669718	–0.457862
6	–1.846729	–2.287961	–0.454709
6	–2.749086	–3.290743	–0.838569
1	–3.807410	–3.050448	–0.878777
6	–2.334125	–4.572430	–1.168669
1	–3.068139	–5.317931	–1.460490
6	–0.983913	–4.919623	–1.127059
1	–0.664589	–5.926620	–1.372792
6	–0.050786	–3.960669	–0.774872
1	1.004175	–4.214241	–0.752687
6	0.813412	–0.297589	–1.671828
6	1.267953	1.031837	–1.612545
6	1.313154	1.734069	–2.821486
1	1.642885	2.767751	–2.822565
6	0.946319	1.150512	–4.028532
1	1.000052	1.728655	–4.945051
6	0.487334	–0.156832	–4.056249
1	0.167282	–0.611687	–4.986789
6	0.409298	–0.877612	–2.873376
1	0.004553	–1.883602	–2.885990
6	3.143944	1.214157	0.319490
6	3.226394	1.126598	1.850064
6	4.612491	0.669018	2.306301
6	5.710167	1.584298	1.763299
6	5.637803	1.696700	0.240341
6	4.252705	2.156766	–0.219047
1	3.383686	0.221991	–0.078914
1	2.470463	0.429614	2.231574
1	2.995590	2.102082	2.296490
1	4.657469	0.629729	3.399626
1	4.783108	–0.353766	1.946124
1	6.695478	1.218097	2.069073
1	5.598109	2.583391	2.204610
1	6.402043	2.389563	–0.126924
1	5.854544	0.718446	–0.207591
1	4.222203	2.199432	–1.314506
1	4.073714	3.178531	0.139717
6	–2.626709	–1.060119	1.711935
6	–4.077817	–1.503299	1.954848
6	–4.388446	–1.763188	3.431150
6	–4.047640	–0.546276	4.291748
6	–2.589397	–0.132433	4.097486
6	–2.274517	0.126497	2.622528
1	–1.996478	–1.895100	2.072004
1	–4.295159	–2.406925	1.373388
1	–4.764962	–0.732285	1.581660
1	–5.442956	–2.033871	3.560330
1	–3.799539	–2.623550	3.777973
1	–4.250598	–0.752221	5.348816
1	–4.700196	0.289929	4.005283
1	–2.361111	0.755440	4.699971
1	–1.939135	–0.937418	4.468445
1	–1.209732	0.360099	2.515978
1	–2.809277	1.026457	2.297182
6	–3.366484	–0.051973	–0.825080
6	–2.833273	0.110702	–2.258105
6	–3.751762	0.911069	–3.181928
6	–4.051688	2.287827	–2.590546
6	–4.645984	2.151729	–1.190046
6	–3.737011	1.332173	–0.271841
1	–4.302798	–0.636153	–0.886352
1	–2.630415	–0.872889	–2.699044
1	–1.863072	0.625612	–2.208739
1	–3.297623	1.014858	–4.175264
1	–4.696079	0.367631	–3.323412
1	–4.724934	2.854686	–3.243595
1	–3.115762	2.861923	–2.530225
1	–4.829821	3.141998	–0.755690
1	–5.624275	1.657354	–1.263700
1	–4.213456	1.237224	0.708212
1	–2.807528	1.894604	–0.102328
6	1.071156	3.013435	0.285532
6	0.027728	2.415749	1.267696
6	–0.757281	3.505258	2.000119
6	–1.424509	4.472602	1.023445
6	–0.406218	5.065953	0.051140
6	0.362935	3.969513	–0.686004
1	1.777239	3.601400	0.891282
1	0.517150	1.770850	2.005443
1	–0.673062	1.779885	0.715212
1	–1.505970	3.037791	2.646780
1	–0.074232	4.063075	2.654405
1	–1.936592	5.269802	1.571924
1	–2.196719	3.938647	0.456534
1	–0.907765	5.719624	–0.669967
1	0.302301	5.696150	0.605458
1	1.088532	4.430823	–1.366095
1	–0.336925	3.401719	–1.311673
1	0.590006	–0.621997	0.957344
1	–1.238139	–0.139172	0.040329

3–CH1

SCF energy = –2102.20725642

5	–2.732985	–0.243708	0.229131
8	–1.502627	0.301337	1.230355
5	2.410540	1.342112	–0.123489
15	0.553390	–1.194889	–0.213382
6	1.765563	–2.481590	0.254974
6	2.753540	–2.954297	–0.607840
1	2.822168	–2.563993	–1.617874
6	3.669607	–3.903828	–0.171864
1	4.439023	–4.258498	–0.849752
6	3.603142	–4.394405	1.126250
1	4.321551	–5.133109	1.465812
6	2.614675	–3.935227	1.989919
1	2.556323	–4.316869	3.003793
6	1.704401	–2.980652	1.557613
1	0.941475	–2.616707	2.239916
6	–0.938372	–2.132826	–0.731062
6	–2.236045	–1.629735	–0.481966
6	–3.291864	–2.419443	–0.975016
1	–4.311419	–2.087172	–0.811455
6	–3.101766	–3.616055	–1.645496
1	–3.960859	–4.178223	–1.998824
6	–1.816234	–4.104555	–1.842367
1	–1.650249	–5.053080	–2.342382
6	–0.746090	–3.362055	–1.378213
1	0.260169	–3.746811	–1.512529
6	1.272203	–0.443448	–1.718041
6	2.164287	0.626778	–1.519698
6	2.796867	1.161398	–2.649111
1	3.508218	1.975235	–2.532611
6	2.515376	0.698840	–3.928395
1	3.004017	1.149583	–4.786277
6	1.602705	–0.332319	–4.107626
1	1.369959	–0.692084	–5.104325
6	0.993869	–0.909708	–3.001855
1	0.283582	–1.718014	–3.139295
1	–0.598318	–0.010271	0.951988
1	–1.503513	1.261640	1.278298
6	–2.958774	0.969989	–0.841056
6	–4.315386	0.891142	–1.560562
6	–4.544682	2.069091	–2.510471
6	–3.415384	2.201049	–3.532691
6	–2.055129	2.283972	–2.840709
6	–1.850008	1.101994	–1.894775
1	–2.974864	1.920702	–0.272347
1	–5.133237	0.843858	–0.834696
1	–4.360258	–0.043051	–2.137132
1	–5.507536	1.960675	–3.021925
1	–4.606992	2.995113	–1.922555
1	–3.577375	3.076428	–4.170849
1	–3.425511	1.324837	–4.194669
1	–1.249242	2.317948	–3.582167
1	–1.996845	3.222107	–2.270757
1	–0.867115	1.189952	–1.423729
1	–1.806536	0.177831	–2.485423
6	–3.935860	–0.454836	1.304122
6	–4.321018	0.841023	2.040294
6	–5.473904	0.642082	3.026311
6	–5.161414	–0.463118	4.034676
6	–4.794091	–1.765412	3.323854
6	–3.646854	–1.560387	2.332762
1	–4.835450	–0.764703	0.749317
1	–4.587174	1.626864	1.324998
1	–3.452617	1.214702	2.603980
1	–5.696224	1.580737	3.546478
1	–6.379827	0.373233	2.466416
1	–6.010995	–0.618400	4.708566
1	–4.317959	–0.147084	4.663843
1	–4.530733	–2.535613	4.057555
1	–5.674112	–2.139080	2.782762
1	–3.430889	–2.503825	1.821082
1	–2.736271	–1.298618	2.889214
6	3.874001	1.260341	0.471018
1	4.456163	1.780952	–0.317861
6	4.420528	–0.183284	0.501637
1	4.267769	–0.661943	–0.468337
1	3.844721	–0.775073	1.224770
6	5.899396	–0.242358	0.879729
1	6.224452	–1.286652	0.934737
1	6.492843	0.231471	0.086134
6	6.170626	0.470370	2.203190
1	7.239836	0.447659	2.437797
1	5.660752	–0.066861	3.013944
6	5.664967	1.911684	2.159755
1	6.243934	2.474899	1.415333
1	5.834385	2.404409	3.122939
6	4.180586	1.975638	1.793766
1	3.866369	3.022943	1.744262
1	3.597465	1.511825	2.599452
6	1.239811	2.306127	0.344335
1	0.317083	1.954489	–0.134098
6	1.530868	3.677001	–0.322018

1	1.702620	3.548808	–1.395887
1	2.451386	4.104377	0.097926
6	0.374239	4.654803	–0.107326
1	0.612623	5.622665	–0.559764
1	–0.511686	4.273427	–0.631107
6	0.050781	4.827497	1.375935
1	–0.800097	5.503480	1.504236
1	0.904017	5.298826	1.881018
6	–0.235828	3.479921	2.038271
1	–1.164399	3.081991	1.597256
1	–0.439981	3.610493	3.105235
6	0.926796	2.503131	1.835534
1	0.709605	1.541677	2.315049
1	1.797392	2.904539	2.359463

3–CH2

SCF energy = –2102.20645189

5	2.762676	0.023577	–0.229921
8	1.350539	0.306885	0.336564
5	–2.452000	0.719579	1.106512
15	–0.187142	–0.963211	–0.550710
6	–1.653474	–1.713159	–1.383976
6	–2.269094	–2.874851	–0.913916
1	–1.885261	–3.370517	–0.027774
6	–3.381779	–3.394077	–1.558936
1	–3.852759	–4.295215	–1.181147
6	–3.903283	–2.749631	–2.675858
1	–4.780715	–3.149272	–3.173031
6	–3.303848	–1.589332	–3.148785
1	–3.709329	–1.080863	–4.016849
6	–2.182745	–1.075919	–2.505715
1	–1.719572	–0.168750	–2.885645
6	1.229298	–1.878745	–1.215597
6	2.520568	–1.347844	–1.064157
6	3.551437	–2.041467	–1.711272
1	4.557625	–1.638780	–1.666099
6	3.328906	–3.214995	–2.412550
1	4.160185	–3.726191	–2.889170
6	2.042240	–3.736511	–2.519012
1	1.859831	–4.653885	–3.068187
6	0.986963	–3.057140	–1.937890
1	–0.017814	–3.441629	–2.063257
6	–0.661523	–1.238976	1.182088
6	–1.699125	–0.504649	1.786284
6	–2.037071	–0.860900	3.097635
1	–2.831760	–0.322336	3.605927
6	–1.383746	–1.881936	3.778240
1	–1.666836	–2.117994	4.798722
6	–0.378302	–2.601561	3.150009
1	0.133333	–3.405210	3.668113
6	–0.023146	–2.284107	1.845266
1	0.767062	–2.839087	1.349496
1	–0.385328	0.316588	–1.061261
1	1.366528	0.290105	1.293794
6	3.775017	–0.140547	1.053248
6	5.272886	–0.197281	0.717715
6	6.151736	–0.202389	1.971079
6	5.790884	–1.366357	2.894714
6	4.302203	–1.353942	3.241802
6	3.433424	–1.317974	1.982337
1	3.636518	0.778986	1.652082
1	5.554788	0.639011	0.070093
1	5.486841	–1.112701	0.150254
1	7.211685	–0.253765	1.697101
1	6.012869	0.744903	2.509266
1	6.396327	–1.336637	3.807437
1	6.032993	–2.311753	2.390354
1	4.049695	–2.224973	3.858362
1	4.083076	–0.466130	3.850472
1	2.379872	–1.289409	2.286252
1	3.558378	–2.260073	1.429081
6	3.156440	1.244026	–1.247494
6	3.376312	2.581802	–0.526033
6	3.766002	3.716694	–1.476928
6	2.745965	3.889661	–2.602364
6	2.503423	2.570444	–3.336646
6	2.125627	1.446827	–2.368825
1	4.107529	0.976296	–1.739789
1	4.145547	2.480607	0.246936
1	2.450330	2.852658	0.002732
1	3.882467	4.657709	–0.926487
1	4.747258	3.490175	–1.915897
1	3.079984	4.660762	–3.305662
1	1.799230	4.247760	–2.178323
1	1.726312	2.699965	–4.099666
1	3.419497	2.284575	–3.870967
1	1.982284	0.514539	–2.928138
1	1.153761	1.689692	–1.913780
6	–4.031605	0.641981	1.070138
1	–4.293680	0.655225	2.147998
6	–4.545812	–0.709552	0.527520
1	–4.040696	–1.539234	1.028770
1	–4.282197	–0.789090	–0.533866

6	–6.059531	–0.859466	0.669797
1	–6.379824	–1.810700	0.231024
1	–6.319981	–0.901762	1.736028
6	–6.802694	0.303551	0.014371
1	–7.882641	0.198146	0.159786
1	–6.627838	0.275885	–1.069512
6	–6.316400	1.642490	0.566949
1	–6.579141	1.711850	1.631278
1	–6.829187	2.470502	0.066330
6	–4.802315	1.795599	0.412822
1	–4.487886	2.756183	0.831410
1	–4.558251	1.827722	–0.656401
6	–1.547589	1.960264	0.738485
1	–0.503401	1.631492	0.688626
6	–1.598003	2.904084	1.972112
1	–1.399437	2.347114	2.895733
1	–2.602210	3.335292	2.075597
6	–0.570374	4.029905	1.824871
1	–0.633781	4.709588	2.681266
1	0.435625	3.592644	1.841390
6	–0.762128	4.803630	0.519408
1	0.019789	5.562748	0.416163
1	–1.718305	5.343048	0.556765
6	–0.756117	3.871018	–0.691947
1	0.233321	3.410809	–0.786562
1	–0.927018	4.439931	–1.611815
6	–1.803860	2.767876	–0.543827
1	–1.781625	2.111460	–1.422864
1	–2.799233	3.220033	–0.528266

3–CH3

SCF energy = –2102.19993517

5	–2.561681	–0.042060	–0.197402
8	–0.628798	0.396425	–0.403773
5	2.225130	–0.658984	0.040602
15	–0.108865	1.464804	0.697411
6	0.730527	2.841797	–0.079642
6	2.069058	3.104039	0.203558
1	2.617098	2.461959	0.881892
6	2.698892	4.178476	–0.408773
1	3.743991	4.376438	–0.199585
6	1.994541	4.983619	–1.295526
1	2.491075	5.820202	–1.775694
6	0.654564	4.726506	–1.570336
1	0.106399	5.359695	–2.258881
6	0.015845	3.658612	–0.960309
1	–1.031078	3.462068	–1.164662
6	–1.727991	1.997272	1.231436
6	–2.790560	1.215887	0.761467
6	–4.076180	1.612812	1.148163
1	–4.935527	1.048081	0.799247
6	–4.278305	2.721364	1.956762
1	–5.287757	3.001804	2.240070
6	–3.200933	3.490779	2.392847
1	–3.366443	4.368393	3.007524
6	–1.916796	3.133673	2.021126
1	–1.070207	3.739645	2.330832
6	0.859737	0.670182	1.961914
6	1.887132	–0.220135	1.584396
6	2.573145	–0.800546	2.665480
1	3.385365	–1.486926	2.451100
6	2.260558	–0.535959	3.988708
1	2.823324	–1.020671	4.780996
6	1.226343	0.339075	4.315344
1	0.974205	0.538846	5.350802
6	0.518760	0.943917	3.296031
1	–0.305451	1.606580	3.537816
1	1.817313	0.252566	–0.714715
1	0.091017	–0.162836	–0.758023
6	–2.543698	–1.489717	0.474705
6	–3.985193	–2.045703	0.489392
6	–4.045775	–3.468384	1.046700
6	–3.439113	–3.546127	2.446814
6	–2.013226	–2.997445	2.456134
6	–1.950374	–1.579524	1.888492
1	–1.954679	–2.156835	–0.170608
1	–4.420640	–2.029218	–0.514669
1	–4.618345	–1.396355	1.111841
1	–5.081408	–3.825195	1.058852
1	–3.490757	–4.135714	0.374303
1	–3.455636	–4.577633	2.813727
1	–4.057338	–2.957978	3.138628
1	–1.601581	–3.013957	3.470601
1	–1.371227	–3.649619	1.850610
1	–0.910120	–1.245706	1.892106
1	–2.494049	–0.898165	2.557824
6	–3.083723	0.119101	–1.697334
6	–2.658112	–1.006855	–2.652776
6	–3.304196	–0.876289	–4.032495
6	–3.030680	0.492481	–4.654909
6	–3.466662	1.620754	–3.720091
6	–2.810081	1.485215	–2.345611
1	–4.182119	0.044392	–1.582427

1	–2.893056	–1.987426	–2.229244
1	–1.566892	–0.984864	–2.770233
1	–2.945123	–1.671787	–4.693830
1	–4.388964	–1.018021	–3.933654
1	–3.535744	0.580854	–5.622347
1	–1.955015	0.588384	–4.854118
1	–3.227378	2.593886	–4.162782
1	–4.558062	1.591257	–3.601194
1	–3.153546	2.292419	–1.688024
1	–1.725425	1.611342	–2.460519
6	3.847221	–0.754260	–0.197926
1	4.264779	–1.514262	0.486364
6	4.553379	0.571214	0.134007
1	4.317820	0.880782	1.160000
1	4.151628	1.351169	–0.529197
6	6.071928	0.520200	–0.041734
1	6.520549	1.493376	0.192205
1	6.493734	–0.198215	0.674374
6	6.444250	0.092938	–1.460405
1	7.531973	0.019383	–1.570792
1	6.108899	0.864058	–2.167612
6	5.778687	–1.235416	–1.815069
1	6.198055	–2.025216	–1.176731
1	6.014270	–1.513532	–2.848950
6	4.261222	–1.189144	–1.612062
1	3.854013	–2.177819	–1.838494
1	3.816568	–0.499440	–2.344541
6	1.349826	–2.039883	–0.287004
1	0.379368	–1.976276	0.236386
6	1.994958	–3.320837	0.263216
1	2.168186	–3.216836	1.339990
1	2.983275	–3.461274	–0.193448
6	1.149852	–4.570334	0.003392
1	1.659934	–5.462925	0.383011
1	0.207658	–4.489266	0.561775
6	0.831295	–4.734735	–1.482330
1	0.199176	–5.614645	–1.644420
1	1.764791	–4.915043	–2.032420
6	0.155706	–3.481786	–2.038672
1	–0.824545	–3.361508	–1.558691
1	–0.037193	–3.595861	–3.111631
6	1.007532	–2.239133	–1.777394
1	0.498186	–1.356763	–2.192931
1	1.928613	–2.314252	–2.362904

3–CTSH1

SCF energy = –2102.19278144

5	2.743820	–0.158740	–0.248700
8	1.507822	0.123477	–1.153108
5	–2.569724	1.133731	0.120770
15	–0.331523	–1.110276	0.554468
6	–1.507585	–2.263710	–0.192641
6	–2.395110	–3.013013	0.579839
1	–2.419237	–2.887207	1.657870
6	–3.277247	–3.890087	–0.034037
1	–3.968084	–4.470435	0.567673
6	–3.285653	–4.011143	–1.419718
1	–3.983310	–4.689736	–1.898785
6	–2.406028	–3.262256	–2.192739
1	–2.413888	–3.356952	–3.273009
6	–1.511976	–2.391632	–1.582093
1	–0.816374	–1.812829	–2.182075
6	1.148008	–1.972491	1.103785
6	2.404676	–1.469777	0.701629
6	3.502047	–2.172672	1.236613
1	4.502062	–1.843253	0.977801
6	3.373149	–3.273671	2.065406
1	4.263184	–3.769341	2.441382
6	2.112988	–3.762991	2.402876
1	2.005456	–4.642188	3.029051
6	1.000665	–3.107808	1.915067
1	0.009487	–3.483547	2.155533
6	–1.202954	–0.284925	1.913944
6	–2.225587	0.628059	1.588045
6	–2.909578	1.221061	2.654914
1	–3.709336	1.927529	2.450784
6	–2.576953	0.954349	3.978049
1	–3.116952	1.447474	4.779791
6	–1.555030	0.064108	4.272891
1	–1.286060	–0.142889	5.302825
6	–0.873225	–0.562713	3.238202
1	–0.067484	–1.252630	3.464168
1	0.293681	–0.195500	–0.463313
1	1.601960	0.977612	–1.575823
6	2.994375	1.171694	0.694304
6	4.347017	1.205307	1.419359
6	4.565408	2.507223	2.195648
6	3.433484	2.765938	3.191186
6	2.071167	2.733687	2.497816
6	1.883590	1.430822	1.720424
1	2.990358	2.038876	0.006264
1	5.167439	1.062118	0.708631
1	4.399555	0.362186	2.123005

1	5.529008	2.485901	2.717542
1	4.614682	3.341692	1.482863
1	3.582545	3.723763	3.701968
1	3.455929	1.989945	3.968308
1	1.266511	2.861661	3.231691
1	2.000490	3.581036	1.801448
1	0.903704	1.450033	1.232811
1	1.849399	0.597429	2.436145
6	3.984530	–0.474656	–1.278939
6	4.342754	0.735753	–2.158089
6	5.484712	0.448647	–3.135976
6	5.170808	–0.760874	–4.015951
6	4.835118	–1.985102	–3.164385
6	3.703933	–1.689537	–2.177334
1	4.896328	–0.703866	–0.704111
1	4.605009	1.598845	–1.536475
1	3.462216	1.037706	–2.747217
1	5.688516	1.328957	–3.756942
1	6.402482	0.250243	–2.565804
1	6.009725	–0.976657	–4.687225
1	4.311052	–0.522574	–4.657582
1	4.570879	–2.832389	–3.808384
1	5.731560	–2.287163	–2.605236
1	3.513572	–2.576899	–1.563124
1	2.776229	–1.503053	–2.734631
6	–4.054734	0.917225	–0.381088
1	–4.613816	1.583791	0.308867
6	–4.582902	–0.507021	–0.110939
1	–4.361549	–0.806732	0.916968
1	–4.046157	–1.207961	–0.760033
6	–6.078807	–0.641583	–0.385181
1	–6.395755	–1.675584	–0.211374
1	–6.637685	–0.017553	0.325077
6	–6.420200	–0.214153	–1.811274
1	–7.498649	–0.283568	–1.986085
1	–5.943001	–0.907083	–2.517159
6	–5.924858	1.205006	–2.086743
1	–6.477896	1.908868	–1.450189
1	–6.139488	1.488477	–3.122376
6	–4.426719	1.347300	–1.807991
1	–4.122798	2.381840	–1.990958
1	–3.871356	0.728062	–2.523933
6	–1.467060	2.051234	–0.546233
1	–0.514182	1.891231	–0.027401
6	–1.884429	3.502219	–0.175456
1	–2.043300	3.590164	0.905435
1	–2.839920	3.748977	–0.656218
6	–0.822079	4.510725	–0.616794
1	–1.150319	5.526873	–0.374909
1	0.097293	4.331111	–0.045252
6	–0.521613	4.389702	–2.110341
1	0.259059	5.100272	–2.398433
1	–1.418061	4.659427	–2.684519
6	–0.101966	2.965089	–2.470265
1	0.846413	2.751939	–1.957751
1	0.097115	2.881027	–3.543076
6	–1.164784	1.947258	–2.049267
1	–0.829769	0.934312	–2.296402
1	–2.066798	2.126042	–2.639724

3–CTSH2

SCF energy = –2102.18460222

5	–2.442555	–0.472252	0.238314
8	–0.856734	–0.248442	0.505517
5	2.060018	1.461633	–0.274743
15	0.426914	–1.085918	–0.434420
6	1.617628	–2.421228	0.018595
6	2.671912	–2.796120	–0.809701
1	2.798503	–2.324808	–1.778843
6	3.574019	–3.766711	–0.388822
1	4.394336	–4.054255	–1.038224
6	3.428420	–4.363330	0.857210
1	4.136624	–5.117027	1.184652
6	2.370444	–3.996510	1.681735
1	2.246825	–4.466224	2.651706
6	1.465107	–3.031214	1.262575
1	0.633076	–2.759899	1.907124
6	–0.973579	–2.171363	–0.977844
6	–2.279249	–1.781227	–0.670705
6	–3.326629	–2.584699	–1.130002
1	–4.351357	–2.317066	–0.887263
6	–3.081091	–3.729536	–1.873491
1	–3.909219	–4.340209	–2.220532
6	–1.772461	–4.112279	–2.159299
1	–1.576983	–5.019347	–2.721877
6	–0.716522	–3.340448	–1.700584
1	0.301377	–3.660442	–1.900664
6	1.004034	–0.258121	–1.943965
6	1.833661	0.852097	–1.727147
6	2.379447	1.479115	–2.852278
1	3.038408	2.333992	–2.726012
6	2.078364	1.042737	–4.135712
1	2.505193	1.553499	–4.993068

6	1.223303	–0.037312	–4.328015
1	0.978232	–0.369500	–5.330953
6	0.683945	–0.690743	–3.230475
1	0.008031	–1.525482	–3.374661
1	1.246102	–0.145654	0.385759
1	–0.580713	0.546823	0.968734
6	–2.965107	0.861004	–0.535641
6	–4.494231	0.876163	–0.692007
6	–5.002371	2.157894	–1.356422
6	–4.330092	2.393082	–2.709023
6	–2.807730	2.384557	–2.575037
6	–2.315208	1.100996	–1.906109
1	–2.709911	1.735613	0.089536
1	–4.981735	0.749722	0.280303
1	–4.801172	0.015484	–1.303342
1	–6.090944	2.119742	–1.476041
1	–4.789595	3.009207	–0.695322
1	–4.672971	3.336418	–3.147948
1	–4.632669	1.597864	–3.403491
1	–2.336736	2.507885	–3.556714
1	–2.496160	3.247507	–1.969589
1	–1.225596	1.141571	–1.820096
1	–2.529854	0.247071	–2.563177
6	–3.097054	–0.752872	1.698725
6	–3.084328	0.482808	2.613862
6	–3.723812	0.224337	3.979071
6	–3.073098	–0.966023	4.682953
6	–3.104784	–2.211536	3.797193
6	–2.462098	–1.942772	2.435364
1	–4.154355	–1.014397	1.525003
1	–3.585130	1.327295	2.129578
1	–2.043420	0.805959	2.780429
1	–3.660267	1.120149	4.607234
1	–4.792923	0.018225	3.836138
1	–3.567013	–1.161848	5.640789
1	–2.027922	–0.718525	4.915907
1	–2.604213	–3.047618	4.299079
1	–4.148155	–2.519024	3.646308
1	–2.510593	–2.842546	1.813183
1	–1.392451	–1.735497	2.590441
6	3.545288	1.434153	0.286213
1	4.062429	2.083186	–0.451087
6	4.205957	0.047930	0.168337
1	4.069405	–0.348033	–0.841482
1	3.691055	–0.650544	0.840232
6	5.691634	0.064467	0.522229
1	6.100097	–0.949960	0.462241
1	6.234094	0.666305	–0.219483
6	5.923939	0.652031	1.912974
1	6.994513	0.690425	2.139354
1	5.468324	–0.007662	2.663313
6	5.307387	2.045070	2.023734
1	5.833487	2.724648	1.339615
1	5.451106	2.447917	3.031875
6	3.818303	2.037542	1.670917
1	3.435253	3.060708	1.723987
1	3.273489	1.461086	2.430331
6	0.886236	2.427491	0.220748
1	–0.035279	2.117956	–0.293779
6	1.160140	3.849814	–0.323110
1	1.360433	3.812235	–1.399362
1	2.059761	4.262840	0.152076
6	–0.031896	4.774312	–0.060492
1	0.188388	5.783885	–0.422571
1	–0.889332	4.412493	–0.641575
6	–0.408914	4.814896	1.421206
1	–1.297162	5.437299	1.567024
1	0.402641	5.292185	1.986620
6	–0.648205	3.412120	1.981246
1	–1.537597	2.976850	1.508591
1	–0.861878	3.462097	3.053726
6	0.564756	2.517267	1.724332
1	0.411221	1.525193	2.175026
1	1.420965	2.926581	2.265545

3–CyO

SCF energy = –2101.05237169

5	2.386358	0.321023	0.260586
8	0.744992	0.249001	0.274020
5	–2.165919	–1.199476	–0.437126
15	0.081643	1.179271	–0.759042
6	–1.219016	2.125514	0.056808
6	–1.956249	3.075422	–0.651620
1	–1.772609	3.237400	–1.709559
6	–2.947659	3.800002	–0.007522
1	–3.519248	4.540350	–0.556175
6	–3.220461	3.561879	1.336548
1	–4.004753	4.121089	1.835426
6	–2.498938	2.604165	2.037861
1	–2.715273	2.414259	3.083287
6	–1.490144	1.889497	1.402631
1	–0.913123	1.148653	1.943588
6	1.471806	2.145875	–1.317745

6	2.618300	1.562948	–0.762086
6	3.838655	2.167888	–1.086260
1	4.758387	1.768069	–0.670089
6	3.890271	3.283491	–1.908119
1	4.849202	3.737887	–2.138226
6	2.724153	3.845443	–2.433554
1	2.778084	4.726877	–3.063379
6	1.498814	3.274851	–2.137340
1	0.584689	3.708358	–2.532708
6	–0.709963	0.295906	–2.124704
6	–1.699563	–0.672355	–1.862365
6	–2.260922	–1.318821	–2.969373
1	–3.031249	–2.069442	–2.814756
6	–1.858749	–1.037129	–4.269568
1	–2.314350	–1.565706	–5.100652
6	–0.880223	–0.083132	–4.504285
1	–0.555905	0.137722	–5.515144
6	–0.307777	0.582424	–3.429857
1	0.475367	1.310413	–3.609862
6	2.871219	–1.131868	–0.275410
6	4.391455	–1.334930	–0.187810
6	4.813870	–2.749451	–0.590588
6	4.314536	–3.106979	–1.990744
6	2.803871	–2.903660	–2.106325
6	2.395811	–1.489459	–1.691291
1	2.414054	–1.872889	0.400737
1	4.752001	–1.122121	0.824088
1	4.893817	–0.615896	–0.851477
1	5.903630	–2.854706	–0.538945
1	4.397441	–3.463228	0.133364
1	4.582867	–4.139323	–2.241266
1	4.819161	–2.465273	–2.725827
1	2.468564	–3.115309	–3.128157
1	2.292612	–3.625270	–1.453740
1	1.308084	–1.398530	–1.767332
1	2.811874	–0.768229	–2.410410
6	2.853884	0.710434	1.767199
6	2.571163	–0.387513	2.802195
6	3.051534	–0.022899	4.208149
6	2.466826	1.310377	4.673493
6	2.768673	2.420778	3.667589
6	2.285459	2.048814	2.264934
1	3.950013	0.836943	1.720534
1	3.031259	–1.332316	2.494924
1	1.489574	–0.576009	2.833288
1	2.794754	–0.818020	4.917626
1	4.147690	0.050156	4.204272
1	2.852582	1.573372	5.664673
1	1.377714	1.206853	4.780127
1	2.311619	3.362736	3.992211
1	3.853128	2.593173	3.638989
1	2.536459	2.853056	1.564753
1	1.188927	1.991394	2.279701
6	–3.685726	–0.965725	–0.058135
1	–4.157388	–1.767749	–0.667520
6	–4.273011	0.365131	–0.566036
1	–4.038629	0.506549	–1.624813
1	–3.787453	1.187193	–0.033532
6	–5.780311	0.476820	–0.345799
1	–6.134051	1.455525	–0.688091
1	–6.298597	–0.274496	–0.957043
6	–6.137812	0.264322	1.123429
1	–7.220487	0.332091	1.271639
1	–5.687314	1.068140	1.721529
6	–5.613911	–1.083092	1.614076
1	–6.129486	–1.887240	1.071442
1	–5.850100	–1.223943	2.674070
6	–4.105743	–1.221346	1.397503
1	–3.791704	–2.218790	1.713998
1	–3.582497	–0.510073	2.049753
6	–1.153101	–2.178260	0.283909
1	–0.173014	–2.059400	–0.192669
6	–1.623430	–3.617690	–0.056459
1	–1.759204	–3.735491	–1.138506
1	–2.601334	–3.809899	0.405157
6	–0.615331	–4.654663	0.443617
1	–0.976926	–5.664529	0.221745
1	0.325414	–4.526982	–0.106661
6	–0.347791	–4.501635	1.941137
1	0.402350	–5.229863	2.265716
1	–1.267440	–4.732082	2.496343
6	0.105716	–3.082059	2.279603
1	1.073840	–2.885993	1.804470
1	0.265030	–2.976795	3.357919
6	–0.905726	–2.043377	1.795472
1	–0.526512	–1.042276	2.009577
1	–1.835075	–2.164842	2.358799

3–CyOH

SCF energy = –2177.49706032

5	–2.408411	0.229577	0.312716
8	–0.861411	–0.396517	0.322346
5	2.282478	0.531595	–0.075283

15	–0.558887	–1.368671	–0.863365	1	–0.861492	1.417640	–1.815540
6	0.105861	–2.927891	–0.230418	1	–2.538963	1.467429	–2.320412
6	1.425000	–3.308919	–0.480896	6	–2.972041	0.026406	1.815949
1	2.056474	–2.696515	–1.113761	6	–2.241861	0.882259	2.862881
6	1.930160	–4.475252	0.081442	6	–2.842057	0.741499	4.263219
1	2.959240	–4.759304	–0.108883	6	–2.886493	–0.719545	4.710923
6	1.116778	–5.268839	0.879886	6	–3.612849	–1.589945	3.685215
1	1.512029	–6.178631	1.318999	6	–2.998793	–1.432554	2.292980
6	–0.206591	–4.904706	1.112490	1	–4.021647	0.367486	1.793857
1	–0.843521	–5.530120	1.728021	1	–2.237596	1.936949	2.570184
6	–0.714839	–3.738872	0.559973	1	–1.185921	0.576503	2.900184
1	–1.746621	–3.457498	0.738290	1	–2.273860	1.341002	4.983103
6	–2.209340	–1.604989	–1.492419	1	–3.862435	1.147818	4.255087
6	–3.072389	–0.755522	–0.787482	1	–3.363688	–0.806037	5.693079
6	–4.432441	–0.852954	–1.103306	1	–1.858743	–1.089396	4.830413
1	–5.146283	–0.223969	–0.579836	1	–3.592216	–2.640606	3.998030
6	–4.884073	–1.751382	–2.058216	1	–4.670450	–1.296955	3.645713
1	–5.945155	–1.811932	–2.280088	1	–3.544936	–2.057489	1.575398
6	–3.996574	–2.598003	–2.726773	1	–1.968360	–1.814227	2.323951
1	–4.365241	–3.309237	–3.457742	6	3.861349	0.264834	0.248626
6	–2.644770	–2.533838	–2.439193	1	4.448979	0.883717	–0.445973
1	–1.947370	–3.206725	–2.929783	6	4.297403	–1.191748	–0.000907
6	0.659108	–0.692418	–1.999089	1	4.059884	–1.486769	–1.028566
6	1.835726	–0.032095	–1.564103	1	3.728989	–1.876279	0.651715
6	2.703338	0.342323	–2.605163	6	5.783005	–1.434508	0.266360
1	3.634115	0.836857	–2.352841	1	6.033278	–2.488419	0.099190
6	2.439373	0.117482	–3.947682	1	6.373336	–0.854494	–0.455118
1	3.156405	0.441108	–4.695627	6	6.165353	–1.011778	1.682868
6	1.264120	–0.510418	–4.335024	1	7.236800	–1.161534	1.852217
1	1.037620	–0.677688	–5.382060	1	5.642518	–1.654748	2.404400
6	0.379613	–0.917012	–3.353687	6	5.779690	0.444656	1.935564
1	–0.551350	–1.390328	–3.646712	1	6.380245	1.092019	1.282441
6	–2.273092	1.766798	–0.190433	1	6.024640	0.728732	2.964780
6	–3.572491	2.564145	0.014258	6	4.294368	0.694816	1.661381
6	–3.423064	4.036774	–0.373310	1	4.077118	1.754910	1.812327
6	–2.930827	4.192769	–1.811629	1	3.697647	0.158133	2.410811
6	–1.642137	3.404184	–2.039462	6	1.696120	2.057569	0.084378
6	–1.809067	1.936650	–1.645327	1	0.785618	2.125917	–0.529406
1	–1.506388	2.235857	0.444441	6	2.671343	3.100384	–0.492352
1	–3.908111	2.496643	1.053959	1	2.918079	2.853735	–1.530697
1	–4.372360	2.118125	–0.595681	1	3.617893	3.070243	0.063644
1	–4.373891	4.564509	–0.237688	6	2.121556	4.526571	–0.438341
1	–2.702707	4.510220	0.307335	1	2.866294	5.232155	–0.823641
1	–2.780222	5.251129	–2.050897	1	1.249634	4.601646	–1.100297
1	–3.704264	3.823686	–2.499034	6	1.711110	4.911201	0.981755
1	–1.324945	3.485760	–3.085183	1	1.285795	5.920441	0.997927
1	–0.839081	3.844858	–1.435257	1	2.603996	4.937184	1.621600

6	0.713059	3.903968	1.548778
1	–0.215176	3.953729	0.965152
1	0.446099	4.167803	2.578220
6	1.258080	2.474789	1.502445
1	0.481060	1.802107	1.877681
1	2.093663	2.388485	2.206273
8	1.540148	–0.314047	1.125390
1	0.552799	–0.241476	1.081029
1	1.801474	–1.236766	1.195721

3–CCI1

SCF energy = –2139.09176082

5	–3.045192	0.466596	–0.069513
5	2.098640	–1.036156	–0.101912
15	–0.121193	1.384678	0.234867
6	1.165071	2.671582	–0.042430
6	1.256910	3.238086	–1.315398
1	0.566948	2.923624	–2.093503
6	2.230124	4.187931	–1.599285
1	2.294356	4.616291	–2.594067
6	3.126520	4.580272	–0.612089
1	3.893341	5.314721	–0.835254
6	3.040231	4.026225	0.659688
1	3.741248	4.325497	1.431941
6	2.067224	3.076702	0.942309
1	2.022722	2.628816	1.929641
6	–1.517798	2.328309	0.958714
6	–2.791303	1.751090	0.820057
6	–3.873617	2.390048	1.436288
1	–4.866806	1.953687	1.364289
6	–3.711208	3.588775	2.118288
1	–4.570291	4.075000	2.569764
6	–2.451281	4.166516	2.218288
1	–2.319577	5.107369	2.742464
6	–1.356792	3.531172	1.647926
1	–0.371503	3.976783	1.737476
6	0.602990	0.446797	1.635535
6	1.577180	–0.534029	1.351339
6	2.161499	–1.168211	2.457212
1	2.946164	–1.899531	2.296130
6	1.778425	–0.904254	3.764528
1	2.253815	–1.433527	4.584531
6	0.789390	0.035515	4.016696
1	0.472752	0.248692	5.032472
6	0.218963	0.715094	2.952076
1	–0.541497	1.462827	3.148759
6	3.738374	–0.834386	–0.290250
6	4.203786	0.602956	–0.027055
6	5.725317	0.744533	–0.057440
6	6.309794	0.213179	–1.365336
6	5.872511	–1.230251	–1.613439
6	4.347382	–1.362725	–1.596493
1	4.148550	–1.458044	0.518703
1	3.818211	0.947973	0.935502
1	3.773213	1.279607	–0.780599
1	6.005009	1.793556	0.088429
1	6.155678	0.185416	0.784168
1	7.402442	0.285329	–1.354680
1	5.963194	0.842457	–2.196119
1	6.271267	–1.591900	–2.567299
1	6.297337	–1.875868	–0.833250
1	4.069072	–2.409316	–1.755519
1	3.946373	–0.805527	–2.455042
6	–3.070023	0.732550	–1.632189
6	–4.560283	0.944125	–2.007949
6	–4.712752	1.366970	–3.470610
6	–4.036465	0.373849	–4.416119
6	–2.566487	0.168454	–4.046999
6	–2.419417	–0.275803	–2.590932
1	–2.574774	1.698923	–1.808521
1	–5.015596	1.701216	–1.358645
1	–5.117774	0.012915	–1.843063
1	–5.773999	1.470151	–3.720987
1	–4.261012	2.358332	–3.603294
1	–4.127848	0.716062	–5.452137
1	–4.558178	–0.590855	–4.358955
1	–2.107491	–0.568113	–4.714758
1	–2.021107	1.109807	–4.196658
1	–1.360154	–0.386724	–2.341984
1	–2.873108	–1.264568	–2.478619
6	–3.497719	–0.843677	0.693883
6	–2.636540	–1.102767	1.950178
6	–3.113880	–2.299386	2.770177
6	–3.223475	–3.558680	1.913111
6	–4.143333	–3.317255	0.717269
6	–3.673430	–2.130080	–0.123996
1	–4.501126	–0.552800	1.069676
1	–2.615168	–0.208446	2.578612
1	–1.598471	–1.276220	1.647100
1	–2.428884	–2.465014	3.608353
1	–4.096760	–2.073935	3.206033
1	–3.587481	–4.400244	2.511534
1	–2.224803	–3.839340	1.553632

1	–4.200558	–4.215578	0.092620
1	–5.161982	–3.125900	1.081317
1	–4.377291	–1.965776	–0.945894
1	–2.716504	–2.387387	–0.586729
6	1.554208	–2.551067	–0.542432
6	0.037329	–2.721634	–0.389207
6	–0.437266	–4.092126	–0.874371
6	0.297062	–5.218064	–0.147460
6	1.812514	–5.057849	–0.268207
6	2.267316	–3.679902	0.220175
1	1.789661	–2.712886	–1.606580
1	–0.501320	–1.928659	–0.922344
1	–0.225678	–2.600873	0.668578
1	–1.517597	–4.199925	–0.733246
1	–0.255525	–4.176187	–1.953931
1	–0.017124	–6.192286	–0.536094
1	0.017840	–5.199700	0.914746
1	2.323524	–5.844029	0.298097
1	2.108429	–5.185742	–1.317917
1	3.354227	–3.592271	0.122381
1	2.038506	–3.597910	1.288720
6	1.579179	–0.245712	–1.370909
8	1.445795	0.068803	–2.448092

3–CCI2

SCF energy = –2139.09555279

5	–1.662929	1.384735	–0.147043
5	1.995028	–0.461698	0.162636
15	–0.327284	–1.222574	–1.334896
6	–1.415838	–2.505385	–0.675374
6	–2.757144	–2.563465	–1.051776
1	–3.160215	–1.836025	–1.748042
6	–3.577712	–3.547690	–0.518681
1	–4.621783	–3.591246	–0.807653
6	–3.064622	–4.463545	0.391520
1	–3.711889	–5.223423	0.815892
6	–1.723927	–4.411554	0.758348
1	–1.323346	–5.129419	1.465161
6	–0.893128	–3.439944	0.220562
1	0.156876	–3.411085	0.492653
6	–1.250453	–0.105341	–2.382295
6	–1.826148	1.007604	–1.735472
6	–2.644894	1.804337	–2.549666
1	–3.119354	2.678554	–2.116221
6	–2.850357	1.532395	–3.893860
1	–3.488840	2.184803	–4.481241
6	–2.229652	0.445073	–4.504646
1	–2.374604	0.247496	–5.560874
6	–1.424039	–0.380364	–3.742504
1	–0.931676	–1.233594	–4.199507
6	1.211604	–1.950856	–1.859199
6	2.274977	–1.552551	–1.023428
6	3.510613	–2.154871	–1.301617
1	4.369318	–1.902851	–0.689206
6	3.663979	–3.071958	–2.329922
1	4.638369	–3.515029	–2.511485
6	2.581555	–3.446874	–3.127626
1	2.710518	–4.173856	–3.921917
6	1.339660	–2.891216	–2.885174
1	0.480340	–3.194236	–3.476331
6	1.875771	–1.157927	1.677998
6	1.734316	–0.110875	2.791860
6	1.510583	–0.757275	4.159492
6	2.629100	–1.745876	4.490291
6	2.785271	–2.795696	3.390086
6	2.996082	–2.152846	2.016016
1	0.945542	–1.754234	1.718367
1	0.914318	0.579784	2.569103
1	2.642769	0.502743	2.833218
1	1.441063	0.011395	4.936675
1	0.546524	–1.284634	4.155029
1	2.441984	–2.230485	5.454607
1	3.573639	–1.195719	4.596614
1	3.614796	–3.472091	3.624633
1	1.877880	–3.415456	3.357333
1	3.053473	–2.936370	1.253281
1	3.966412	–1.640513	2.001046
6	–2.694980	0.471309	0.737643
6	–4.072300	1.138636	0.880225
6	–5.090792	0.198732	1.529873
6	–4.590666	–0.322829	2.877977
6	–3.216923	–0.981020	2.745766
6	–2.200651	–0.035014	2.103858
1	–2.895185	–0.441050	0.162583
1	–4.439614	1.456428	–0.103498
1	–3.987884	2.051803	1.481972
1	–6.054986	0.704225	1.653208
1	–5.267128	–0.653724	0.859209
1	–5.312871	–1.027786	3.304268
1	–4.520254	0.515515	3.583781
1	–2.859281	–1.313402	3.726758
1	–3.304066	–1.882500	2.123398

1	–1.246374	–0.563628	2.001632
1	–2.003519	0.805172	2.779369
6	–1.572555	2.979258	0.140307
6	–0.491354	3.664656	–0.718563
6	–0.374152	5.166859	–0.461795
6	–0.115973	5.453004	1.016158
6	–1.198216	4.815698	1.885432
6	–1.322609	3.313149	1.622362
1	–2.543432	3.431301	–0.123539
1	–0.672509	3.488155	–1.784010
1	0.478533	3.200852	–0.496742
1	0.425491	5.592741	–1.078279
1	–1.305168	5.663280	–0.768520
1	–0.061264	6.531878	1.197579
1	0.861739	5.037373	1.295480
1	–0.989961	4.995196	2.946118
1	–2.161269	5.299191	1.671174
1	–2.124377	2.909533	2.246875
1	–0.399632	2.817435	1.951189
6	2.864649	0.924045	0.041291
6	2.767817	1.530312	–1.370418
6	3.433609	2.902435	–1.466915
6	4.894698	2.837217	–1.022073
6	5.022958	2.225949	0.373812
6	4.341567	0.856111	0.454336
1	2.383585	1.643430	0.723897
1	1.720402	1.617511	–1.686493
1	3.242388	0.848781	–2.090438
1	3.363393	3.293030	–2.488274
1	2.889394	3.608768	–0.825388
1	5.349029	3.833585	–1.045412
1	5.458960	2.220865	–1.735267
1	6.079127	2.142578	0.654088
1	4.556679	2.898483	1.106165
1	4.442705	0.457017	1.468285
1	4.880618	0.162203	–0.205020
6	0.475065	–0.060364	–0.107059
8	–0.158167	0.918254	0.276911

3–CCI3

SCF energy = –2139.07805309

5	–1.148360	1.660535	–0.350893
5	1.961109	–0.741155	–0.030075
15	–0.474117	–1.318114	–1.105855
6	–1.885736	–2.257954	–0.472865
6	–3.182931	–1.963545	–0.893240
1	–3.352285	–1.190500	–1.634183
6	–4.258441	–2.656114	–0.353328
1	–5.265521	–2.417889	–0.676729
6	–4.045914	–3.639632	0.604101
1	–4.889990	–4.168693	1.033188
6	–2.752294	–3.951322	1.009286
1	–2.582258	–4.727255	1.747471
6	–1.673193	–3.269101	0.468415
1	–0.666427	–3.532662	0.771923
6	–1.028913	–0.166127	–2.354625
6	–1.309223	1.141001	–1.909323
6	–1.834925	1.990966	–2.895463
1	–2.069696	3.015968	–2.628456
6	–2.045935	1.581060	–4.203237
1	–2.449594	2.283635	–4.926103
6	–1.729653	0.284845	–4.605697
1	–1.879384	–0.027927	–5.633262
6	–1.216369	–0.596135	–3.672604
1	–0.958027	–1.610697	–3.963465
6	0.842273	–2.453333	–1.535956
6	2.046452	–2.069912	–0.916312
6	3.154104	–2.884229	–1.151073
1	4.107914	–2.639113	–0.697895
6	3.055650	–4.018084	–1.951228
1	3.934422	–4.632126	–2.120886
6	1.842982	–4.382998	–2.528353
1	1.775904	–5.275537	–3.140809
6	0.717532	–3.598301	–2.314339
1	–0.238751	–3.879174	–2.745411
6	0.921210	–1.201046	1.646925
6	1.178013	–0.145571	2.714794
6	0.658902	–0.638122	4.068566
6	1.301694	–1.970698	4.454425
6	1.104011	–3.020107	3.360647
6	1.610637	–2.529300	1.997568
1	–0.152615	–1.412482	1.666368
1	0.694097	0.792359	2.438912
1	2.250068	0.054594	2.800512
1	0.856743	0.116324	4.836237
1	–0.431455	–0.754337	4.019194
1	0.893702	–2.334404	5.402855
1	2.377120	–1.818277	4.614504
1	1.613989	–3.952242	3.625761
1	0.034344	–3.257232	3.277709
1	1.430690	–3.294501	1.239161
1	2.696859	–2.395501	2.038093
6	–2.516889	1.222307	0.455151

6	–3.665335	2.224679	0.264723
6	–4.974648	1.722762	0.878736
6	–4.796744	1.371585	2.356640
6	–3.660984	0.367036	2.554567
6	–2.353959	0.876259	1.943299
1	–2.886583	0.292832	0.000336
1	–3.814491	2.428035	–0.802663
1	–3.401853	3.186204	0.723403
1	–5.767342	2.470340	0.760085
1	–5.304784	0.826091	0.335266
1	–5.731745	0.980306	2.773274
1	–4.565463	2.288075	2.916088
1	–3.526968	0.152367	3.621424
1	–3.931196	–0.583969	2.073931
1	–1.580043	0.113375	2.064483
1	–2.003144	1.747279	2.508548
6	–0.698918	3.228165	–0.269817
6	0.605669	3.489264	–1.045416
6	1.079253	4.941421	–0.977547
6	1.239279	5.401082	0.470542
6	–0.056073	5.187682	1.251396
6	–0.532633	3.735401	1.172728
1	–1.486781	3.850158	–0.727075
1	0.497430	3.188082	–2.093421
1	1.388758	2.846188	–0.624283
1	2.025378	5.058050	–1.519175
1	0.348137	5.588574	–1.481667
1	1.544619	6.452716	0.511818
1	2.044851	4.822033	0.943353
1	0.077670	5.485820	2.297841
1	–0.834527	5.843721	0.837775
1	–1.475285	3.644072	1.719869
1	0.189200	3.093493	1.695709
6	3.145307	0.281276	0.237091
6	3.550760	0.884960	–1.125496
6	4.564402	2.016961	–0.957822
6	5.797992	1.553313	–0.181432
6	5.416006	0.922201	1.158442
6	4.399931	–0.207280	0.975190
1	2.724189	1.111945	0.820843
1	2.664000	1.254808	–1.650720
1	3.982664	0.100095	–1.762119
1	4.859068	2.410674	–1.936474
1	4.082998	2.845375	–0.421480
1	6.487204	2.389596	–0.024498
1	6.341734	0.812149	–0.783108
1	6.310803	0.550171	1.669277
1	4.979883	1.690658	1.810128
1	4.143927	–0.631191	1.952170
1	4.878516	–1.017547	0.409463
6	0.544610	–0.226506	–0.027666
8	0.089449	0.933631	0.290903

3–CCO

SCF energy = –2139.12412932

5	1.639777	–1.057949	0.120234
5	–0.079622	1.536953	–0.309255
15	–1.304031	–0.326591	1.244568
6	–3.079082	–0.552299	1.457981
6	–3.678831	–1.738410	1.026295
1	–3.068546	–2.559339	0.664952
6	–5.059385	–1.862513	1.053425
1	–5.524278	–2.780762	0.712335
6	–5.844232	–0.809596	1.512811
1	–6.924236	–0.909302	1.530768
6	–5.249276	0.366950	1.950595
1	–5.861696	1.186494	2.309901
6	–3.866921	0.500970	1.921062
1	–3.402261	1.425826	2.245631
6	–0.427396	–1.808312	1.731251
6	0.836353	–2.015248	1.158224
6	1.520199	–3.154805	1.616036
1	2.505502	–3.364538	1.212980
6	0.998887	–4.006509	2.572973
1	1.573416	–4.868907	2.896890
6	–0.255783	–3.761911	3.129353
1	–0.666245	–4.425314	3.882850
6	–0.969653	–2.657705	2.707440
1	–1.948034	–2.454941	3.132323
6	–0.708292	1.118076	2.117257
6	–0.080940	2.002249	1.229825
6	0.512860	3.132719	1.794648
1	1.020625	3.849841	1.158988
6	0.487236	3.345541	3.167466
1	0.965588	4.226714	3.583137
6	–0.128375	2.433066	4.022361
1	–0.130634	2.604204	5.093307
6	–0.728120	1.298927	3.496515
1	–1.194915	0.568342	4.150614
6	–1.627598	–0.485877	–1.590927
6	–0.882113	–0.532687	–2.931729
6	–1.680637	–1.356543	–3.940650
6	–3.075685	–0.764055	–4.154834

6	–3.818395	–0.569710	–2.831285
6	–2.979371	0.210926	–1.818677
1	–1.836776	–1.535792	–1.326962
1	0.119961	–0.933359	–2.807849
1	–0.761770	0.481066	–3.322345
1	–1.141668	–1.405815	–4.891824
1	–1.764266	–2.390287	–3.579490
1	–3.662817	–1.396118	–4.828844
1	–2.972921	0.209969	–4.650518
1	–4.770963	–0.058509	–3.003064
1	–4.065908	–1.550226	–2.402575
1	–3.540498	0.327521	–0.889480
1	–2.784934	1.223731	–2.191583
6	2.083863	–1.835378	–1.260548
6	1.145459	–2.990267	–1.659787
6	1.439872	–3.536945	–3.056047
6	2.889971	–4.012026	–3.152377
6	3.862452	–2.909351	–2.732734
6	3.533906	–2.345428	–1.346692
1	2.006828	–1.065988	–2.044317
1	0.095036	–2.690610	–1.584315
1	1.258134	–3.809386	–0.937968
1	0.754666	–4.356539	–3.301955
1	1.264848	–2.750076	–3.802733
1	3.117106	–4.355850	–4.167400
1	3.023878	–4.879566	–2.491946
1	4.891234	–3.286507	–2.755498
1	3.814512	–2.092535	–3.465414
1	4.241608	–1.544962	–1.113384
1	3.707104	–3.130977	–0.597030
6	2.858963	–0.302956	0.898943
6	2.644289	0.079190	2.374095
6	3.912477	0.648013	3.013377
6	4.443657	1.847871	2.229054
6	4.676391	1.483645	0.762473
6	3.405545	0.910504	0.135482
1	3.663985	–1.056669	0.915117
1	2.305449	–0.788238	2.949792
1	1.854299	0.829291	2.458703
1	3.716599	0.931930	4.053978
1	4.685504	–0.132278	3.042361
1	5.365227	2.228925	2.683073
1	3.706727	2.661227	2.282017
1	5.015537	2.362355	0.201614
1	5.481280	0.738862	0.697506
1	3.582775	0.660859	–0.916795
1	2.642274	1.695031	0.134590
6	0.034807	2.581199	–1.510478
6	1.420436	3.199820	–1.758152
6	1.404063	4.182897	–2.931086
6	0.345548	5.270089	–2.744493
6	–1.038320	4.660327	–2.518789
6	–1.023685	3.687849	–1.339154
1	–0.219782	2.058267	–2.439577
1	2.148630	2.407897	–1.951861
1	1.776109	3.724684	–0.861498
1	2.393492	4.634732	–3.060746
1	1.190785	3.630497	–3.856226
1	0.331535	5.942444	–3.608999
1	0.611865	5.886989	–1.875185
1	–1.780199	5.449672	–2.354116
1	–1.348445	4.123899	–3.425854
1	–2.016486	3.240740	–1.207029
1	–0.825433	4.251546	–0.418106
6	–0.851544	0.149961	–0.445083
8	0.589961	0.112520	–0.464610

4–3MAu

SCF energy = –1365.50620045

79	–0.758284	–1.290413	–0.064959
17	–0.979732	–3.605406	–0.093249
7	–0.517742	1.633794	–0.122415
5	0.309042	0.504506	–0.063786
5	–1.568580	0.691663	–0.046866
6	–3.147370	0.754068	0.158186
6	–3.347029	0.866460	1.686975
1	–2.923139	0.004504	2.210669
1	–4.417859	0.896544	1.916290
1	–2.893091	1.769669	2.103783
6	–3.811284	1.952771	–0.537206
1	–4.890804	1.932314	–0.353368
1	–3.667641	1.920118	–1.621330
1	–3.446694	2.914761	–0.175753
6	–3.871351	–0.514674	–0.330364
1	–3.558828	–1.412846	0.206872
1	–3.705207	–0.694575	–1.396344
1	–4.950579	–0.403661	–0.178103
6	–0.274332	3.090409	–0.157888
6	–0.816082	3.641631	–1.478988
1	–0.635753	4.717808	–1.539537
1	–1.886964	3.471708	–1.583883
1	–0.312242	3.166737	–2.324916
6	–0.956859	3.743658	1.045230

1	–0.576133	3.319454	1.978210
1	–2.037965	3.609061	1.027422
1	–0.753800	4.817201	1.053360
6	1.228771	3.363387	–0.082670
1	1.399440	4.441938	–0.118835
1	1.767225	2.909601	–0.916393
1	1.666646	2.983567	0.842425
6	1.848743	0.284501	0.007524
6	2.482318	0.196878	1.255444
6	3.857649	0.004294	1.305596
1	4.349600	–0.059958	2.273204
6	4.619609	–0.116373	0.146086
6	3.971183	–0.039590	–1.082933
1	4.551046	–0.137453	–1.997510
6	2.596777	0.152646	–1.170091
6	1.910444	0.217438	–2.510375
1	1.373409	1.163336	–2.642956
1	1.175203	–0.587715	–2.616029
1	2.621865	0.125501	–3.332746
6	1.672865	0.307749	2.522291
1	2.303687	0.252844	3.411119
1	0.934358	–0.498548	2.589259
1	1.120986	1.253457	2.567717
6	6.102662	–0.363627	0.224148
1	6.550486	0.150177	1.078130
1	6.614286	–0.026047	–0.679835
1	6.309913	–1.432110	0.340450

4–3MAuCy

SCF energy = –2412.71296790

79	0.266957	–0.394793	–0.136819
17	1.961545	–2.272148	1.861840
15	–2.082240	–0.216585	0.031965
7	3.329371	–0.605543	–0.033673
5	2.263637	–1.646431	0.063372
5	2.315618	0.294115	–0.165928
6	3.191314	–3.900494	–0.805158
1	4.196354	–3.487447	–0.915760
1	3.096267	–4.713797	–1.535483
1	3.119868	–4.339105	0.193681
6	2.095823	–2.842613	–1.033503
6	2.241016	–2.284261	–2.456631
1	1.442500	–1.570372	–2.688399
1	2.188286	–3.089809	–3.199318
1	3.190107	–1.762506	–2.599622
6	0.743907	–3.570950	–0.941464
1	0.562110	–3.957718	0.064390
1	0.716551	–4.418271	–1.638343
1	–0.092682	–2.912332	–1.202694
6	5.255205	–1.477042	1.206131
1	6.340130	–1.406337	1.326450
1	5.005097	–2.511279	0.962716
1	4.782719	–1.242817	2.161990
6	4.785928	–0.510425	0.116938
6	5.465040	–0.845999	–1.216090
1	5.123446	–0.167463	–2.002531
1	5.250925	–1.867125	–1.533395
1	6.550229	–0.741847	–1.125592
6	5.163922	0.919880	0.509637
1	4.690440	1.208007	1.450947
1	4.859694	1.641056	–0.252041
1	6.246956	0.998426	0.637841
6	2.153907	1.855506	–0.229413
6	2.114506	2.514021	–1.470683
6	1.840930	3.875312	–1.520072
1	1.810267	4.377392	–2.485012
6	1.603346	4.614204	–0.362033
6	1.643606	3.951309	0.858421
1	1.455055	4.508972	1.773556
6	1.902520	2.584661	0.941746
6	1.831120	1.888294	2.276495
1	1.993663	2.583706	3.103211
1	2.557192	1.076675	2.363264
1	0.844611	1.430114	2.415626
6	2.339542	1.729401	–2.736712
1	1.580910	0.946471	–2.850106
1	3.308913	1.222618	–2.726519
1	2.302197	2.367148	–3.622504
6	1.298597	6.086838	–0.446597
1	1.154995	6.525096	0.543674
1	0.388398	6.270234	–1.026575
1	2.110061	6.632867	–0.936649
6	–1.855253	–0.192665	2.795973
1	–2.017059	0.889194	2.777283
1	–0.782113	–0.351950	2.636034
6	–2.237702	–0.757720	4.163271
1	–1.654957	–0.255428	4.941213
1	–3.294149	–0.540221	4.370199
6	–2.004951	–2.266551	4.211912
1	–2.298447	–2.668208	5.186538
1	–0.933724	–2.468650	4.092935
6	–2.775855	–2.969486	3.096184
1	–3.854125	–2.849999	3.267501

1	–2.573680	–4.044546	3.111080
6	–2.417647	–2.406108	1.719694
1	–3.019090	–2.909657	0.956930
1	–1.366599	–2.631928	1.499267
6	–2.631510	–0.883836	1.660585
1	–3.701001	–0.671200	1.779652
6	–2.949637	–1.203877	–1.257647
1	–2.597924	–2.225385	–1.063418
6	–4.479793	–1.196215	–1.182721
1	–4.847450	–0.179577	–1.368998
1	–4.821247	–1.477660	–0.181268
6	–5.080595	–2.139803	–2.227213
1	–4.792272	–3.171634	–1.989006
1	–6.173139	–2.101632	–2.176679
6	–4.599115	–1.788728	–3.635354
1	–5.005094	–2.498724	–4.362191
1	–4.989290	–0.800704	–3.912865
6	–3.072201	–1.768024	–3.713345
1	–2.745620	–1.467047	–4.713265
1	–2.683354	–2.781071	–3.550634
6	–2.465029	–0.831255	–2.667363
1	–2.748840	0.202951	–2.900503
1	–1.372366	–0.874135	–2.714270
6	–2.696780	1.527653	–0.119448
1	–2.935405	1.625695	–1.187404
6	–1.587798	2.549965	0.192150
1	–1.255865	2.431876	1.230887
1	–0.706078	2.360595	–0.425074
6	–2.067278	3.983441	–0.026396
1	–2.251525	4.140749	–1.097429
1	–1.267232	4.673588	0.254815
6	–3.343358	4.284151	0.757216
1	–3.127483	4.239942	1.832859
1	–3.688540	5.301824	0.550481
6	–4.441616	3.274380	0.425391
1	–4.728521	3.383036	–0.628780
1	–5.341020	3.476610	1.015374
6	–3.973365	1.839300	0.676688
1	–4.772501	1.136291	0.426854
1	–3.778144	1.717234	1.747951

4–3MAuDMA

SCF energy = –1747.75319835

79	0.285826	–0.768646	–1.311609
17	–0.141017	–1.173504	–3.600355
7	0.435863	–0.208964	1.565192
7	–1.942800	–0.162563	0.594795
7	–5.320696	2.175869	–0.181427
5	1.182291	–0.006353	0.421998
5	–0.546371	–1.019171	0.765918
6	0.555942	0.222759	2.968006
6	1.337179	–0.807316	3.791929
1	2.326039	–0.973445	3.359176
1	0.820056	–1.765876	3.846103
1	1.475796	–0.446145	4.815139
6	1.303913	1.557434	3.035969
1	2.316491	1.473511	2.639474
1	1.369439	1.898022	4.073019
1	0.780498	2.328787	2.464856
6	–0.838499	0.413083	3.576776
1	–0.751728	0.650820	4.640289
1	–1.448968	–0.486504	3.484182
1	–1.374401	1.236312	3.097031
6	–3.165321	–0.705601	0.476682
1	–3.227963	–1.775136	0.575118
6	–1.868850	1.178481	0.479339
1	–0.880508	1.598468	0.582096
6	–4.303601	0.020620	0.236590
1	–5.237921	–0.515879	0.153721
6	–4.233328	1.421948	0.087480
6	–2.944496	1.984923	0.237396
1	–2.770221	3.047340	0.143907
6	–5.187577	3.613112	–0.343151
1	–4.788947	4.080086	0.562548
1	–6.166703	4.045558	–0.535447
1	–4.534610	3.864465	–1.185037
6	–6.613406	1.543063	–0.374443
1	–6.946478	1.028817	0.532605
1	–6.585958	0.822046	–1.197257
1	–7.352678	2.302181	–0.619009
6	2.541788	0.742866	0.149134
6	2.569758	2.082555	–0.277180
6	3.788127	2.718660	–0.481875
1	3.796222	3.757707	–0.805063
6	4.999630	2.059597	–0.293246
6	4.961178	0.724344	0.087787
1	5.895402	0.181987	0.214819
6	3.757010	0.056622	0.298160
6	3.769411	–1.414219	0.624049
1	4.776249	–1.767568	0.856119
1	3.399973	–1.995355	–0.227470
1	3.123365	–1.656202	1.469813
6	1.290912	2.841709	–0.524841

1	0.765947	3.059239	0.412075
1	0.611431	2.272289	–1.167773
1	1.483363	3.798044	–1.015186
6	6.305346	2.769107	–0.537364
1	7.151884	2.194279	–0.155431
1	6.322255	3.750511	–0.055251
1	6.470628	2.929282	–1.607442
6	–0.735217	–2.635138	1.014970
6	–1.520156	–2.945872	2.307984
1	–0.992401	–2.589343	3.194985
1	–1.640560	–4.028921	2.427108
1	–2.523662	–2.511433	2.344406
6	–1.374521	–3.410903	–0.160236
1	–1.499149	–4.465360	0.113735
1	–0.738177	–3.382101	–1.047962
1	–2.352859	–3.050912	–0.484577
6	0.658017	–3.267863	1.192392
1	0.562906	–4.345436	1.370107
1	1.206276	–2.842189	2.032692
1	1.271080	–3.135938	0.297554

4–3MAuMe

SCF energy = –1826.64092614

79	0.924715	–0.601591	0.038915
17	1.385399	1.901271	–1.964881
15	2.604142	–2.268203	–0.045823
7	–0.841941	1.890158	–0.170774
5	–0.912003	0.532273	–0.000380
5	0.636787	1.773552	–0.214867
6	–2.103445	–0.490778	0.068913
6	–2.706552	–0.796162	1.298203
6	–3.756500	–1.708203	1.343095
1	–4.224347	–1.932051	2.299603
6	–4.224487	–2.337874	0.193513
6	–3.598426	–2.047331	–1.015254
1	–3.942540	–2.539898	–1.922489
6	–2.543436	–1.143660	–1.093182
6	–2.211318	–0.138641	2.560348
1	–2.361914	0.944551	2.533216
1	–1.135975	–0.299608	2.692419
1	–2.721470	–0.524751	3.445437
6	–5.392773	–3.287031	0.250635
1	–6.336796	–2.757823	0.083605
1	–5.463547	–3.778885	1.223928
1	–5.316244	–4.064194	–0.513940
6	–1.852799	–0.898012	–2.411001
1	–2.454067	–1.247293	–3.253463
1	–0.890961	–1.423349	–2.447664
1	–1.627015	0.159644	–2.569781
6	–1.829961	2.960457	–0.378008
6	–3.160802	2.362740	–0.841081
1	–3.879592	3.165141	–1.028821
1	–3.588954	1.693467	–0.092806
1	–3.038127	1.797395	–1.767416
6	–1.319917	3.929068	–1.447947
1	–1.174385	3.414583	–2.399694
1	–0.365010	4.377171	–1.168185
1	–2.044952	4.734655	–1.595367
6	1.617111	2.399196	0.926809
6	1.036713	2.166669	2.328724
1	0.031342	2.580194	2.433645
1	1.670316	2.631956	3.093554
1	0.971194	1.097689	2.559553
6	1.743632	3.917092	0.690508
1	2.162746	4.134468	–0.295512
1	2.406988	4.364318	1.441016
1	0.783921	4.432515	0.765161
6	3.044086	1.825787	0.898573
1	3.489784	1.898865	–0.096715
1	3.061883	0.772562	1.201353
1	3.689324	2.371125	1.598258
6	2.153379	–3.796710	–0.926583
1	1.862664	–3.548157	–1.948825
1	1.296187	–4.259612	–0.434671
1	2.984432	–4.506120	–0.950497
6	3.236180	–2.853310	1.558383
1	2.420992	–3.303248	2.127597
1	3.616791	–2.001813	2.125478
1	4.035491	–3.587376	1.429254
6	4.088963	–1.675113	–0.913581
1	3.813825	–1.371595	–1.925058
1	4.864198	–2.444167	–0.957501
1	4.475202	–0.794176	–0.397944
6	–2.064908	3.708994	0.939168
1	–2.823393	4.485703	0.804694
1	–1.155420	4.189087	1.301526
1	–2.417725	3.022898	1.713351

4–3MAuMeI

SCF energy = –1826.63519489

79	–0.351488	–1.370371	–0.167322
17	–0.696939	–3.703110	–0.075547

15	–2.527727	0.347661	1.320851
7	–0.187210	1.553508	0.023075
5	0.651597	0.465052	–0.024602
5	–1.345863	0.638960	–0.318802
6	2.213625	0.273270	0.039370
6	2.986398	0.271418	–1.134335
6	4.368184	0.124501	–1.050599
1	4.954238	0.128448	–1.966809
6	5.015880	–0.042535	0.167673
6	4.236437	–0.089330	1.318956
1	4.718611	–0.253771	2.279875
6	2.854266	0.052407	1.271300
6	2.334969	0.379984	–2.488096
1	1.802405	1.325415	–2.614664
1	1.602165	–0.419002	–2.633436
1	3.070963	0.306065	–3.290864
6	6.514763	–0.163225	0.241442
1	6.979271	0.817341	0.389397
1	6.928385	–0.585731	–0.677177
1	6.824504	–0.800501	1.073183
6	2.052650	–0.077631	2.539821
1	2.697260	–0.144375	3.418392
1	1.436857	–0.983957	2.510438
1	1.380064	0.770633	2.683997
6	0.067394	2.998622	0.154427
6	1.168421	3.231254	1.194769
1	1.367681	4.301537	1.295665
1	2.099754	2.738277	0.914116
1	0.865693	2.856723	2.176313
6	–1.191571	3.725199	0.630829
1	–1.488867	3.380690	1.625325
1	–2.030336	3.587898	–0.049830
1	–0.997828	4.797811	0.707973
6	–2.194535	0.714195	–1.722022
6	–1.245312	0.542489	–2.918148
1	–0.430108	1.268424	–2.894399
1	–1.784728	0.682020	–3.862551
1	–0.799572	–0.455495	–2.939376
6	–2.918396	2.059756	–1.915520
1	–3.602114	2.301308	–1.096193
1	–3.521195	2.031402	–2.830972
1	–2.221345	2.892308	–2.025379
6	–3.268676	–0.383789	–1.820673
1	–4.084622	–0.227884	–1.105542
1	–2.863036	–1.386413	–1.657535
1	–3.729233	–0.375907	–2.814851
6	–1.561843	0.569585	2.838436
1	–1.056581	1.534640	2.829825
1	–0.806144	–0.214152	2.889592
1	–2.210269	0.502360	3.713981
6	–3.304669	–1.280199	1.554914
1	–2.542967	–2.051517	1.672356
1	–3.912133	–1.543809	0.690622
1	–3.936140	–1.251319	2.446285
6	–3.942011	1.485585	1.507075
1	–3.622400	2.523384	1.421345
1	–4.416950	1.336087	2.479425
1	–4.675964	1.282760	0.725763
6	0.535959	3.571426	–1.187466
1	0.692184	4.651412	–1.113372
1	–0.190248	3.386925	–1.980493
1	1.484378	3.114768	–1.477903

4–3MAuPh

SCF energy = –2401.76277392

79	–0.209672	–0.504812	–0.063130
17	–1.946815	–2.371283	1.934688
5	–2.223977	0.274672	–0.014794
5	–2.265232	–1.683352	0.173968
15	2.133484	–0.195871	0.002301
7	–3.271679	–0.580226	0.136318
6	–2.003112	1.829228	–0.065404
6	–2.004663	2.505232	–1.295761
6	–1.701279	3.862287	–1.337036
1	–1.702813	4.376933	–2.295439
6	–1.386703	4.574006	–0.182698
6	–1.374218	3.889317	1.029127
1	–1.118055	4.426169	1.940248
6	–1.669160	2.530888	1.105129
6	–2.292372	1.746399	–2.564265
1	–1.528100	0.980584	–2.738675
1	–2.314336	2.404702	–3.435216
1	–3.250986	1.222950	–2.510440
6	–1.555141	1.809379	2.424122
1	–0.568815	1.340050	2.523921
1	–2.288035	1.005035	2.521521
1	–1.682034	2.492060	3.267386
6	–1.085120	6.049037	–0.237272
1	–0.741333	6.352982	–1.229449
1	–0.316216	6.328658	0.487891
1	–1.977544	6.640012	–0.007370
6	–2.188199	–2.842853	–0.968101
6	–2.337292	–2.228605	–2.367543

1	–2.341052	–3.010496	–3.136670
1	–1.509723	–1.547048	–2.595095
1	–3.262329	–1.656601	–2.471448
6	–0.876046	–3.644716	–0.933551
1	–0.901653	–4.452774	–1.675369
1	–0.703521	–4.095060	0.046776
1	–0.005097	–3.022128	–1.168200
6	–3.333271	–3.849618	–0.748922
1	–4.318322	–3.385693	–0.835831
1	–3.270503	–4.316942	0.237382
1	–3.287647	–4.648022	–1.499884
6	–4.717541	–0.418426	0.335083
6	–5.449739	–0.666834	–0.988752
1	–5.292106	–1.682198	–1.353699
1	–5.101375	0.028116	–1.757612
1	–6.525837	–0.518244	–0.860523
6	–5.205627	–1.403513	1.399171
1	–6.284555	–1.293449	1.541394
1	–4.709135	–1.221318	2.354126
1	–5.001722	–2.437579	1.116006
6	–5.011489	1.011442	0.795620
1	–4.699900	1.747584	0.051606
1	–4.493349	1.238449	1.730386
1	–6.084574	1.135221	0.965244
6	2.753090	–0.163712	1.711386
6	2.181990	–1.049248	2.629454
1	1.370336	–1.704950	2.326422
6	2.638002	–1.082320	3.939901
1	2.187513	–1.770508	4.646551
6	3.655424	–0.225687	4.345514
1	4.004914	–0.246715	5.372435
6	4.215885	0.666566	3.439366
1	5.000693	1.344835	3.756855
6	3.768526	0.698791	2.124164
1	4.203472	1.404494	1.424331
6	3.126021	–1.454653	–0.855141
6	4.305203	–1.974467	–0.324163
1	4.663517	–1.636658	0.642536
6	5.018741	–2.938011	–1.027878
1	5.932005	–3.344363	–0.606591
6	4.560292	–3.384837	–2.260647
1	5.115848	–4.141494	–2.804447
6	3.382570	–2.870551	–2.792912
1	3.014023	–3.226175	–3.748891
6	2.665009	–1.913273	–2.091485
1	1.736791	–1.525836	–2.501636
6	2.625752	1.394200	–0.733213
6	3.855738	1.562892	–1.370872
1	4.540503	0.726475	–1.466795
6	4.202571	2.801081	–1.896568
1	5.158139	2.925466	–2.394801
6	3.325554	3.874594	–1.789615
1	3.596217	4.838620	–2.207608
6	2.097705	3.709830	–1.159751
1	1.397870	4.534624	–1.083636
6	1.744537	2.474080	–0.635343
1	0.774486	2.357689	–0.161570

AuClPCy3

SCF energy = –1642.92276086

79	2.004613	0.003685	–0.005640
15	–0.264541	0.001175	0.004944
6	–0.891628	–0.448569	–1.676213
6	–2.363737	–0.865090	–1.811304
6	–0.513635	0.652195	–2.684924
1	–0.280589	–1.328197	–1.920417
6	–2.693961	–1.255957	–3.254568
1	–3.026352	–0.053994	–1.496819
1	–2.579334	–1.711753	–1.157531
6	–0.862405	0.239362	–4.115129
1	–1.047871	1.578907	–2.443944
1	0.554357	0.878103	–2.610192
6	–2.335195	–0.146369	–4.240594
1	–3.756305	–1.507066	–3.329467
1	–2.138916	–2.165805	–3.516542
1	–0.618741	1.055093	–4.802131
1	–0.235230	–0.612006	–4.407376
1	–2.560203	–0.462245	–5.263745
1	–2.960282	0.734333	–4.041151
6	–0.883714	1.683178	0.462378
6	–2.351783	2.019162	0.164701
6	–0.510235	1.999151	1.922608
1	–0.266498	2.333337	–0.172941
6	–2.668199	3.468349	0.544565
1	–3.021665	1.347429	0.709425
1	–2.565566	1.878156	–0.896563
6	–0.845546	3.447231	2.280847
1	–1.056388	1.331489	2.599333
1	0.554765	1.809093	2.086562
6	–2.313373	3.766400	2.000066
1	–3.727265	3.671504	0.358943
1	–2.101177	4.142515	–0.110176
1	–0.607761	3.628138	3.333287

1	–0.206051	4.119592	1.695792
1	–2.525870	4.813793	2.234491
1	–2.949591	3.162452	2.660789
6	–0.875186	–1.237964	1.233600
6	–2.342619	–1.158621	1.681117
6	–0.498568	–2.655541	0.764267
1	–0.254398	–1.016140	2.112282
6	–2.650395	–2.225699	2.735767
1	–3.015469	–1.288235	0.829410
1	–2.558906	–0.173752	2.100247
6	–0.824608	–3.701378	1.830023
1	–1.046562	–2.901817	–0.152701
1	0.565948	–2.696839	0.512752
6	–2.291766	–3.628562	2.249702
1	–3.709340	–2.173211	3.007988
1	–2.083125	–2.003648	3.648653
1	–0.583443	–4.698549	1.450096
1	–0.184504	–3.536617	2.705119
1	–2.501312	–4.365301	3.030796
1	–2.928309	–3.891402	1.394154
17	4.313231	0.005073	–0.017555

AuClPMe3

SCF energy = –1056.86774730

79	–0.559507	0.000478	–0.002627
15	1.689775	–0.000184	0.000121
6	2.449860	–1.606680	–0.382063
6	2.442453	0.467307	1.587768
6	2.457664	1.137012	–1.192649
17	–2.859508	–0.000649	0.004594
1	2.113042	–0.225316	2.363652
1	3.533234	0.447445	1.522347
1	2.114007	1.470040	1.865466
1	2.129722	–1.936754	–1.371782
1	3.540021	–1.535784	–0.358318
1	2.118951	–2.348084	0.346791
1	2.131664	2.157129	–0.984062
1	3.547564	1.084660	–1.131966
1	2.137995	0.876882	–2.202859

AuClPPh3

SCF energy = –1631.97899336

15	0.400488	0.000222	0.010647
6	1.112837	–1.570047	0.592128
6	0.489823	–2.222986	1.673048
1	–0.411222	–1.806726	2.105023
6	1.025918	–3.397942	2.166871
1	0.534319	–3.900568	3.002589
6	2.164711	–3.948659	1.607576
1	2.578980	–4.871537	1.988112
6	2.786131	–3.305712	0.523046
1	3.669825	–3.736754	0.077772
6	2.254263	–2.124777	0.029881
1	2.737177	–1.637842	–0.817653
6	1.158211	1.281427	1.054060
6	0.569547	2.539892	1.114235
1	–0.368145	2.724485	0.585457
6	1.149438	3.561953	1.841634
1	0.684621	4.535443	1.887987
6	2.350312	3.325765	2.535878
1	2.802018	4.124566	3.106024
6	2.931718	2.072112	2.486085
1	3.859588	1.884611	3.029672
6	2.353837	1.047676	1.756488
1	2.813157	0.068622	1.729203
6	1.133844	0.251707	–1.636713
6	2.319397	0.977947	–1.815458
1	2.801757	1.447670	–0.969340
6	2.864073	1.103665	–3.085840
1	3.783869	1.671969	–3.219473
6	2.248249	0.518213	–4.177801
1	2.672942	0.624115	–5.169670
6	1.062705	–0.204767	–4.005269
1	0.572047	–0.654131	–4.856030
6	0.513747	–0.330312	–2.737941
1	–0.416586	–0.880593	–2.609135
79	–1.855735	0.028448	0.007194
17	–4.155949	0.041469	–0.007647

AuClSMe2

SCF energy = –1073.75539510

79	0.397053	–0.000004	–0.084879
6	–2.536823	1.385744	0.476096
1	–2.136308	2.300042	0.041078
6	–2.536838	–1.385727	0.476106
1	–2.236099	–1.315471	1.520079
17	2.642216	0.000008	0.280623
1	–3.623201	1.381752	0.384101
1	–2.236094	1.315487	1.520072
1	–2.136342	–2.300033	0.041090

1	–3.623216	–1.381718	0.384120
16	–1.865727	0.000001	–0.479304

BNBMes

SCF energy = –769.712209283

7	1.199052	0.587277	–0.008712
6	1.383581	2.003174	0.327759
6	2.816405	2.425735	0.015684
1	3.534257	1.849951	0.604089
1	2.961315	3.484407	0.246638
6	1.086838	2.164106	1.821071
1	0.048914	1.896414	2.034374
1	1.242609	3.200626	2.132487
1	1.740339	1.522611	2.418348
6	3.156901	–1.400414	–0.247658
6	2.981777	–2.895857	–0.551713
6	3.802722	–1.245173	1.141891
1	3.173907	–1.671444	1.930445
1	3.984839	–0.196245	1.393240
1	4.767309	–1.765506	1.175223
5	0.183331	–0.371682	–0.187317
5	1.752614	–0.688076	–0.223898
1	3.949316	–3.413006	–0.542856
1	2.334259	–3.379356	0.185374
1	3.041149	2.275524	–1.043197
6	0.393794	2.828439	–0.495144
1	–0.631982	2.498154	–0.313548
1	0.467175	3.887239	–0.232950
1	0.604182	2.728870	–1.563353
6	4.077033	–0.777454	–1.310524
1	3.639370	–0.844860	–2.311748
1	4.284171	0.275704	–1.107163
1	5.038202	–1.304661	–1.338489
1	2.526776	–3.051350	–1.534272
6	–1.367835	–0.374055	–0.132362
6	–2.135678	–0.062072	–1.265774
6	–2.017835	–0.711940	1.064377
6	–3.523616	–0.073631	–1.180394
6	–3.409049	–0.711539	1.117107
6	–4.180691	–0.388921	0.005975
1	–4.110835	0.162041	–2.065599
1	–3.903824	–0.978758	2.048300
6	–1.455614	0.270059	–2.569746
1	–0.703381	–0.482563	–2.827746
1	–2.170152	0.323562	–3.393797
1	–0.940643	1.233975	–2.515697
6	–1.211185	–1.085917	2.283016
1	–1.844600	–1.486330	3.077369
1	–0.458603	–1.843084	2.039017
1	–0.674944	–0.224035	2.693258
6	–5.685029	–0.369604	0.081101
1	–6.059416	0.650394	0.216578
1	–6.135820	–0.762664	–0.833817
1	–6.052093	–0.967384	0.918554

DMAP

SCF energy = –382.205679337

7	–2.661695	0.000011	0.025211
7	1.551363	0.000011	–0.099953
6	–1.948753	–1.125814	0.011911
1	–2.522072	–2.050227	0.029762
6	–1.948736	1.125820	0.011766
1	–2.522086	2.050213	0.029480
6	–0.566591	–1.192051	–0.018760
1	–0.090206	–2.163620	–0.018807
6	0.181393	–0.000028	–0.046390
6	–0.566599	1.192025	–0.018949
1	–0.090214	2.163596	–0.019170
6	2.270510	1.247515	0.038470
1	1.988551	1.954891	–0.746955
1	3.338725	1.060806	–0.061103
1	2.095848	1.726934	1.010920
6	2.270538	–1.247492	0.038185
1	1.987932	–1.954971	–0.746917
1	2.096577	–1.726725	1.010846
1	3.338703	–1.060896	–0.062254

PCy3

SCF energy = –1047.13579636

15	0.014259	–0.128844	–1.064029
6	2.732400	–0.289416	–0.502756
1	2.731657	0.795918	–0.363089
1	2.860332	–0.457259	–1.579815
6	3.912339	–0.906607	0.249586
1	4.850572	–0.466361	–0.103190
1	3.831870	–0.660224	1.316629
6	3.939137	–2.425069	0.081441
1	4.766698	–2.859737	0.651094
1	4.123719	–2.666182	–0.973535
6	2.611530	–3.044366	0.514991
1	2.479992	–2.895498	1.594877

1	2.623121	–4.126594	0.349508
6	1.423190	–2.420520	–0.221922
1	0.498286	–2.866187	0.155644
1	1.480247	–2.673135	–1.289373
6	1.388987	–0.893548	–0.061807
1	1.244128	–0.672998	1.002578
6	–1.495309	–1.035570	–0.449501
1	–1.302666	–2.076441	–0.744215
6	–1.776616	–1.015610	1.056536
1	–1.970432	0.016284	1.374339
1	–0.901336	–1.357188	1.618513
6	–2.993188	–1.873461	1.413808
1	–2.773767	–2.925307	1.187636
1	–3.185836	–1.819988	2.490343
6	–4.230182	–1.434812	0.629930
1	–5.080844	–2.081755	0.867015
1	–4.512550	–0.420680	0.942718
6	–3.962300	–1.438799	–0.875344
1	–4.841342	–1.077083	–1.418520
1	–3.791884	–2.470495	–1.209589
6	–2.739653	–0.590227	–1.233999
1	–2.961150	0.462668	–1.013379
1	–2.542433	–0.646009	–2.308979
6	–0.194741	1.575313	–0.299651
1	–1.284614	1.717232	–0.270460
6	0.364601	2.649754	–1.247946
1	1.450141	2.518633	–1.349125
1	–0.051082	2.510086	–2.250142
6	0.068998	4.063912	–0.744489
1	–1.016082	4.231832	–0.767068
1	0.511122	4.802611	–1.420978
6	0.579270	4.272463	0.680681
1	1.675750	4.212279	0.684481
1	0.321245	5.275097	1.036547
6	0.017795	3.210574	1.625710
1	–1.070132	3.334978	1.708061
1	0.423626	3.345946	2.633757
6	0.331306	1.797712	1.125735
1	–0.084206	1.059745	1.816060
1	1.418580	1.658136	1.146071

PMe3

SCF energy = –461.089520157

15	0.007780	0.005388	–0.608509
6	1.598605	0.239432	0.286771
1	2.294069	–0.547927	–0.018904
1	2.051417	1.196171	0.013122
1	1.491524	0.214406	1.375278
6	–0.596075	–1.510604	0.276522
1	–1.632402	–1.724288	0.005293
1	0.014780	–2.370330	–0.016459
1	–0.548556	–1.392444	1.362790
6	–1.016092	1.264529	0.279210
1	–0.701090	2.272549	–0.006981
1	–2.062745	1.142269	–0.007562
1	–0.942328	1.168623	1.366045

4–3NAuCy

SCF energy = –2354.97298879

7	–3.134183	1.573399	0.481750
15	2.266465	0.157733	0.036580
6	–2.724650	2.830205	1.139753
1	–3.644754	3.376480	1.361796
6	–1.904979	3.732564	0.217313
1	–0.934378	3.284184	–0.008244
1	–1.734557	4.705777	0.688724
1	–2.427884	3.896642	–0.728512
6	–4.590389	1.421344	0.308868
1	–4.730167	0.458258	–0.179614
6	–5.348873	1.363066	1.637488
1	–6.414108	1.199398	1.451481
1	–5.258077	2.290729	2.210486
1	–4.992347	0.543444	2.262949
79	–0.089491	0.588658	0.156657
5	–2.197536	0.618930	0.023057
7	–2.740784	–0.595944	–0.727010
6	–2.721297	–0.429721	–2.230683
6	–4.121168	–0.629337	–2.828427
1	–4.536556	–1.610656	–2.617082
1	–4.075454	–0.509992	–3.915302
1	–4.810960	0.126474	–2.442855
6	–1.689706	–1.385296	–2.848981
1	–1.947425	–2.433340	–2.712356
1	–1.596094	–1.195903	–3.922900
1	–0.713596	–1.207721	–2.387313
6	–2.280282	0.990243	–2.640458
1	–2.384935	1.083242	–3.724550
1	–2.889801	1.767273	–2.181681
1	–1.237913	1.192145	–2.388223
5	–2.985481	–1.785967	–0.038982
17	–3.615159	–3.259763	–0.951345
6	–2.697902	–2.159500	1.511323

6	–3.874534	–2.944832	2.124124
1	–4.089644	–3.869277	1.587546
1	–4.791414	–2.345153	2.133341
1	–3.646470	–3.208319	3.163675
6	–1.445157	–3.066276	1.490565
1	–1.603087	–3.979371	0.912063
1	–1.176275	–3.359596	2.512990
1	–0.585962	–2.537125	1.065123
6	–2.393853	–1.011593	2.485658
1	–2.233426	–1.423914	3.489302
1	–3.209004	–0.292588	2.552574
1	–1.494726	–0.455061	2.217703
6	–5.192682	2.493666	–0.604171
1	–6.251460	2.284191	–0.781357
1	–5.128967	3.494105	–0.165774
1	–4.693133	2.521754	–1.574118
6	–2.030670	2.602679	2.481397
1	–1.856861	3.559594	2.983704
1	–2.643561	1.978030	3.135209
1	–1.066148	2.106903	2.348277
6	3.287817	1.654273	–0.328863
6	3.192539	2.670650	0.821206
6	3.929580	3.970808	0.494959
6	3.430120	4.586467	–0.810513
6	3.550831	3.587619	–1.959291
6	2.807053	2.289498	–1.646218
1	4.337492	1.353570	–0.442609
1	3.601986	2.247568	1.743026
1	2.134788	2.888639	1.017977
1	3.809342	4.677446	1.321876
1	5.005280	3.767868	0.411147
1	3.985909	5.501160	–1.038364
1	2.378371	4.877621	–0.693816
1	3.158510	4.019619	–2.885017
1	4.611041	3.367454	–2.140905
1	2.923934	1.589545	–2.478479
1	1.732234	2.497880	–1.565926
6	1.866529	–2.335300	–1.199723
6	2.516824	–0.960628	–1.418578
6	3.929939	–1.115791	–1.996353
1	1.909711	–0.451531	–2.180991
6	1.819800	–3.126542	–2.506310
1	0.857922	–2.222197	–0.790484
1	2.446649	–2.902119	–0.461895
6	3.212578	–3.269798	–3.120176
1	1.375656	–4.110197	–2.327921
1	1.157376	–2.611186	–3.212832
6	3.881749	–1.907213	–3.307026
1	3.153137	–3.795217	–4.078159
1	3.835936	–3.889846	–2.462413
1	4.894158	–2.031186	–3.704164
1	3.322434	–1.328283	–4.053547
1	4.391977	–0.140471	–2.173158
1	4.574535	–1.640116	–1.284596
6	2.987983	–0.581933	1.569757
1	3.049373	0.285370	2.241095
6	2.023313	–1.574796	2.240881
1	1.874925	–2.448479	1.598374
1	1.038694	–1.116200	2.365656
6	2.563544	–2.034094	3.595623
1	2.581312	–1.179911	4.285012
1	1.880731	–2.770144	4.030619
6	3.971783	–2.616505	3.475685
1	4.351269	–2.900829	4.461956
1	3.933615	–3.537620	2.879339
6	4.925663	–1.625513	2.808000
1	5.049323	–0.746498	3.453824
1	5.918795	–2.070616	2.691522
6	4.393880	–1.179533	1.443925
1	4.357268	–2.052103	0.782409
1	5.083541	–0.463888	0.984566

4–3NI1

SCF energy = –2354.94422718

7	–3.203551	–0.791813	–0.345749
5	–2.181134	–1.435384	0.357815
6	–1.890442	–2.896068	0.947067
6	–1.014421	–2.811226	2.211113
1	–0.033383	–2.384214	1.993883
1	–0.860936	–3.811721	2.632714
1	–1.476072	–2.192207	2.986718
6	–1.125112	–3.719139	–0.106555
1	–0.163558	–3.256048	–0.348293
1	–1.680228	–3.825277	–1.041739
1	–0.921508	–4.725563	0.277993
6	–3.177707	–3.636136	1.347428
1	–3.827121	–3.853056	0.499027
1	–3.759430	–3.063079	2.076141
1	–2.928440	–4.596770	1.812596
6	–4.424776	–1.139357	–1.096352
6	–5.574625	–1.400804	–0.120649
1	–6.500384	–1.591112	–0.670935
1	–5.376316	–2.260134	0.520357

6	–4.114730	–2.370011	–1.951892
1	–3.300001	–2.143382	–2.643996
1	–4.994607	–2.653758	–2.535028
1	–3.825447	–3.229946	–1.349196
5	–2.549479	0.324837	0.261447
1	–5.735537	–0.529104	0.519102
6	–4.797674	0.003934	–2.042884
1	–3.917603	0.359005	–2.584648
1	–5.534881	–0.351156	–2.767798
1	–5.251225	0.838188	–1.507127
79	–0.396431	–0.135570	0.254762
15	1.942156	0.012038	–0.071133
6	2.254957	–0.160733	–1.872781
6	3.637496	0.213895	–2.421500
6	1.806089	–1.553307	–2.346940
1	1.519412	0.547295	–2.280311
6	3.647178	0.110509	–3.949628
1	4.415264	–0.437409	–2.008672
1	3.898324	1.234901	–2.134034
6	1.836600	–1.638795	–3.872379
1	2.455502	–2.330498	–1.921206
1	0.788172	–1.748651	–1.996460
6	3.213945	–1.275117	–4.425721
1	4.645359	0.351550	–4.329180
1	2.961602	0.862065	–4.359613
1	1.549473	–2.645850	–4.191292
1	1.081941	–0.950408	–4.269554
1	3.204862	–1.312367	–5.519472
1	3.950230	–2.020049	–4.093575
6	2.774194	–1.335808	0.875504
6	4.221122	–1.699992	0.518999
6	2.611646	–1.089076	2.384785
1	2.151239	–2.206309	0.623961
6	4.695287	–2.898244	1.347252
1	4.885431	–0.847795	0.694233
1	4.300122	–1.942592	–0.542713
6	3.082446	–2.298279	3.191440
1	3.198030	–0.211054	2.681598
1	1.567306	–0.859192	2.618853
6	4.526953	–2.661277	2.847834
1	5.741284	–3.117300	1.111547
1	4.117722	–3.784960	1.055067
1	2.982200	–2.093197	4.261596
1	2.426880	–3.151287	2.973755
1	4.840048	–3.548176	3.407165
1	5.189453	–1.844128	3.162558
6	2.534372	1.658831	0.513497
6	4.039089	1.876683	0.723493
6	1.927438	2.758077	–0.378443
1	2.057886	1.744667	1.499819
6	4.297816	3.273001	1.298790
1	4.578156	1.764928	–0.222133
1	4.446332	1.126667	1.405887
6	2.191331	4.140497	0.213841
1	2.372860	2.707245	–1.378461
1	0.856546	2.594725	–0.528041
6	3.686755	4.373022	0.430351
1	5.374801	3.430196	1.414319
1	3.864970	3.328514	2.306384
1	1.775760	4.907356	–0.446409
1	1.663667	4.231170	1.172404
1	3.859941	5.352393	0.887063
1	4.192893	4.388291	–0.543657
17	–1.054819	1.145994	–2.314222
7	–2.857148	1.620886	0.723443
6	–3.623223	2.548728	–0.122637
6	–5.031641	2.783253	0.424921
1	–3.693977	2.065283	–1.093688
1	–5.550532	1.834893	0.586661
1	–5.623645	3.381380	–0.273964
1	–5.015008	3.319340	1.379073
1	–3.457359	4.467312	–1.087043
6	–2.882706	3.858896	–0.383485
1	–1.911629	3.649700	–0.835725
1	–2.745649	4.453344	0.525374
6	–2.394538	2.136013	2.020837
1	–3.034259	2.995626	2.241358
6	–2.623054	1.121005	3.140286
1	–1.975865	0.248231	3.017165
1	–3.661292	0.779588	3.147248
1	–2.399218	1.566923	4.113726
6	–0.948169	2.641820	2.036561
1	–0.244314	1.804208	1.991834
1	–0.741513	3.300338	1.193480
1	–0.748539	3.190446	2.962813

4–3NI2

SCF energy = –2354.96236343

7	–2.972866	1.613143	0.463432
15	2.097669	0.308817	–0.110483
6	–2.166934	2.805374	0.761834
1	–2.875656	3.573599	1.078906
6	–1.500764	3.352838	–0.499184

1	–0.805097	2.623972	–0.921997	1	–0.344655	2.011825	1.696541
1	–0.946288	4.273692	–0.288820	6	2.566062	1.824720	–1.058232
1	–2.253069	3.568221	–1.261585	6	2.237610	3.110353	–0.284272
6	–4.381492	1.745652	0.851165	6	2.503404	4.364745	–1.120137
1	–4.862989	0.835192	0.518638	6	1.785540	4.318686	–2.467643
6	–4.555520	1.793581	2.371415	6	2.170667	3.060296	–3.241487
1	–5.617393	1.793871	2.636512	6	1.867616	1.801971	–2.429726
1	–4.110354	2.694211	2.805678	1	3.650775	1.793638	–1.220040
1	–4.084653	0.922761	2.834043	1	2.831816	3.164014	0.632502
79	–0.296155	0.041857	0.087195	1	1.187859	3.093045	0.024926
5	–2.463300	0.345599	0.018681	1	2.198065	5.249718	–0.552974
7	–3.104829	–0.802737	–0.493913	1	3.583469	4.462865	–1.291282
6	–4.378379	–1.163754	–1.143999	1	2.021158	5.214062	–3.051030
6	–4.163397	–2.364911	–2.075500	1	0.700782	4.324915	–2.305106
1	–3.448338	–2.126557	–2.863274	1	1.637567	3.017084	–4.195817
1	–5.114432	–2.639068	–2.541270	1	3.241833	3.092453	–3.481174
1	–3.786913	–3.238491	–1.542918	1	2.163320	0.915085	–2.997005
6	–4.846051	–0.002290	–2.031500	1	0.784219	1.717571	–2.284090
1	–4.048151	0.279384	–2.722868	6	2.717728	–2.417460	–0.348773
1	–5.717288	–0.306271	–2.619115	6	2.765963	–1.092175	–1.120601
1	–5.128064	0.882747	–1.465502	6	4.130777	–0.906430	–1.798410
6	–5.477092	–1.548747	–0.137434	1	2.005980	–1.168607	–1.909910
1	–6.413358	–1.758910	–0.663650	6	3.007230	–3.594770	–1.278268
1	–5.201738	–2.446628	0.417084	1	1.740499	–2.544118	0.118232
1	–5.681592	–0.768145	0.596664	1	3.465066	–2.404212	0.454074
5	–1.919276	–1.620881	–0.153638	6	4.353973	–3.425534	–1.981112
17	–0.926067	–2.381923	–1.631396	1	2.987688	–4.528798	–0.708556
6	–1.894488	–2.609181	1.146758	1	2.202969	–3.664286	–2.020199
6	–2.664781	–3.907920	0.847701	6	4.427130	–2.091028	–2.723695
1	–2.237673	–4.438468	–0.007933	1	4.529361	–4.252362	–2.676130
1	–3.720879	–3.729628	0.638429	1	5.158856	–3.467718	–1.235062
1	–2.621130	–4.582710	1.711951	1	5.412042	–1.962136	–3.183643
6	–0.482672	–3.028342	1.576970	1	3.696820	–2.093594	–3.542871
1	0.020614	–3.591246	0.787067	1	4.163084	0.019547	–2.378890
1	–0.526208	–3.670414	2.465730	1	4.921394	–0.830427	–1.044943
1	0.141227	–2.166242	1.831524	6	2.978223	0.458951	1.506757
6	–2.566311	–1.902086	2.334187	1	2.705398	1.473287	1.827355
1	–2.581527	–2.552052	3.217794	6	2.412638	–0.487814	2.577618
1	–3.598986	–1.621871	2.109296	1	2.580703	–1.531054	2.292775
1	–2.031001	–0.984433	2.603825	1	1.329171	–0.357174	2.651739
6	–5.108683	2.912646	0.172832	6	3.059789	–0.223500	3.937970
1	–6.190410	2.790397	0.280791	1	2.766531	0.774806	4.288386
1	–4.853821	3.880915	0.612853	1	2.673905	–0.936578	4.672506
1	–4.876083	2.956895	–0.893349	6	4.584398	–0.304798	3.865039
6	–1.189813	2.661945	1.933610	1	5.024572	–0.084253	4.842222
1	–0.789295	3.643502	2.208541	1	4.880219	–1.332051	3.614732
1	–1.692434	2.238708	2.805702	6	5.137134	0.649909	2.807217

1	4.929517	1.685771	3.105701
1	6.225354	0.556593	2.737760
6	4.508037	0.382426	1.438429
1	4.804848	–0.617823	1.105124
1	4.898645	1.089167	0.698950

4–3NTS1

SCF energy = –2354.92830250

7	–3.482680	–0.828094	–0.111269
5	–2.409401	–1.323176	0.633514
6	–1.886659	–2.695023	1.239839
6	–1.053868	–2.388433	2.493788
1	–0.250568	–1.689424	2.260586
1	–0.609176	–3.303724	2.905042
1	–1.662540	–1.933751	3.281907
6	–0.994086	–3.431265	0.226660
1	–0.091494	–2.857274	0.000823
1	–1.507080	–3.618265	–0.720603
1	–0.676117	–4.398522	0.635192
6	–3.039945	–3.623093	1.652802
1	–3.618202	–3.973747	0.795278
1	–3.730093	–3.129805	2.344217
1	–2.645752	–4.511153	2.161621
6	–4.651080	–1.292218	–0.874764
6	–5.733785	–1.751879	0.105862
1	–6.622395	–2.082382	–0.439712
1	–5.389113	–2.578646	0.727793
6	–4.187662	–2.443236	–1.771123
1	–3.400173	–2.095677	–2.444307
1	–5.020244	–2.819417	–2.372024
1	–3.796702	–3.274373	–1.181306
5	–2.763025	0.271091	0.461946
1	–6.026089	–0.929016	0.764293
6	–5.207673	–0.175246	–1.755617
1	–4.425241	0.239814	–2.393725
1	–5.998421	–0.575346	–2.396393
1	–5.647733	0.623574	–1.154757
79	–0.339369	0.040109	–0.516361
15	1.920142	–0.023205	–0.083576
6	2.731832	–0.759583	–1.577365
6	4.236436	–0.523126	–1.771807
6	2.358262	–2.247180	–1.698202
1	2.210590	–0.237396	–2.390885
6	4.729890	–1.153434	–3.076795
1	4.807251	–0.933231	–0.933839
1	4.445610	0.547689	–1.797659
6	2.883864	–2.854842	–2.998799
1	2.766656	–2.809289	–0.849246
1	1.271241	–2.356482	–1.656679
6	4.388463	–2.639591	–3.150987
1	5.809382	–1.000056	–3.171919
1	4.264763	–0.634967	–3.924939
1	2.642565	–3.921733	–3.028461
1	2.362068	–2.392332	–3.845460
1	4.740718	–3.063947	–4.096044
1	4.917016	–3.175336	–2.350845
6	2.410101	–0.966227	1.432675
6	3.864001	–1.440841	1.570419
6	1.944086	–0.194055	2.681036
1	1.786259	–1.867432	1.361448
6	4.059096	–2.237002	2.864165
1	4.552869	–0.590615	1.559723
1	4.137193	–2.071968	0.722167
6	2.157949	–1.005705	3.957560
1	2.498054	0.747222	2.767475
1	0.890059	0.079874	2.579531
6	3.614383	–1.446598	4.093183
1	5.109061	–2.531352	2.957367
1	3.478571	–3.166778	2.804412
1	1.852900	–0.412199	4.824836
1	1.508771	–1.889539	3.939618
1	3.748241	–2.045718	4.998885
1	4.253993	–0.561230	4.206727
6	2.504446	1.724861	0.105195
6	3.925900	1.988042	0.624355
6	2.223676	2.520306	–1.182280
1	1.816229	2.111592	0.866820
6	4.145047	3.489085	0.836741
1	4.673445	1.611165	–0.078847
1	4.097498	1.466699	1.567814
6	2.458577	4.014433	–0.961074
1	2.882064	2.169336	–1.986300
1	1.199076	2.347048	–1.524157
6	3.867073	4.288347	–0.435437
1	5.167596	3.665663	1.184828
1	3.477948	3.838018	1.635994
1	2.285120	4.555171	–1.895986
1	1.719868	4.389026	–0.240745
1	4.003976	5.357786	–0.248200
1	4.600430	4.010020	–1.203763
17	–1.615173	0.642909	–2.545442
7	–2.899040	1.644066	0.720711
6	–3.759343	2.486102	–0.120047

6	–5.074206	2.829483	0.580794
1	–3.981944	1.884640	–0.997602
1	–5.582243	1.919051	0.910796
1	–5.744377	3.371052	–0.093283
1	–4.914938	3.460725	1.460961
1	–3.698638	4.266431	–1.335698
6	–3.041293	3.726485	–0.648860
1	–2.147652	3.430278	–1.202157
1	–2.757859	4.423520	0.146112
6	–2.242307	2.296600	1.861710
1	–2.807746	3.213603	2.055326
6	–2.327331	1.444850	3.126600
1	–1.761304	0.517670	3.006685
1	–3.364725	1.182267	3.348675
1	–1.915798	1.986698	3.983507
6	–0.790820	2.700140	1.596398
1	–0.165380	1.805531	1.564970
1	–0.680140	3.220718	0.644158
1	–0.415222	3.347989	2.395464

4–3NTS2

SCF energy = –2354.93863522

7	3.344727	–0.554973	0.184856
5	2.286354	–1.297100	–0.383467
6	2.143515	–2.658835	–1.228740
6	0.861023	–2.680488	–2.085549
1	–0.039864	–2.709339	–1.465866
1	0.850166	–3.579975	–2.712813
1	0.789312	–1.812999	–2.749451
6	2.114095	–3.922733	–0.354498
1	1.286560	–3.885284	0.355948
1	3.023489	–4.060361	0.228463
1	1.992437	–4.806670	–0.992986
6	3.329147	–2.713953	–2.213755
1	4.291114	–2.816453	–1.709863
1	3.376673	–1.815518	–2.839351
1	3.221362	–3.574390	–2.884219
6	4.691846	–0.812800	0.724398
6	5.733180	–0.436832	–0.332429
1	6.743427	–0.559675	0.068186
1	5.637759	–1.064496	–1.220957
6	4.812231	–2.286713	1.107596
1	4.003368	–2.566923	1.786466
1	5.768020	–2.460098	1.608297
1	4.781238	–2.937649	0.235138
5	2.519675	0.505684	–0.236328
1	5.612380	0.603339	–0.643427
6	4.902048	0.012241	1.999215
1	4.041632	–0.094049	2.664134
1	5.789204	–0.347848	2.525859
1	5.068327	1.067181	1.782053
79	0.402947	–0.183348	–0.252826
15	–1.939623	0.032725	0.057785
6	–2.422174	–1.082988	1.440487
6	–3.759570	–0.837774	2.151603
6	–2.267763	–2.546774	0.987725
1	–1.612201	–0.910538	2.161610
6	–3.939224	–1.822956	3.311058
1	–4.599231	–0.936923	1.455288
1	–3.800343	0.180869	2.545137
6	–2.455578	–3.501195	2.164801
1	–3.001558	–2.786659	0.207482
1	–1.270124	–2.694986	0.565918
6	–3.799847	–3.274036	2.853951
1	–4.913611	–1.659201	3.782942
1	–3.179557	–1.614383	4.074360
1	–2.373798	–4.534535	1.813473
1	–1.634137	–3.341527	2.871633
1	–3.908296	–3.949201	3.708416
1	–4.615192	–3.516642	2.158131
6	–2.850945	–0.449909	–1.473627
6	–4.360525	–0.706017	–1.366924
6	–2.524117	0.520682	–2.619708
1	–2.375303	–1.408369	–1.724166
6	–4.922135	–1.195960	–2.704583
1	–4.884930	0.206078	–1.066244
1	–4.566404	–1.450836	–0.596421
6	–3.102711	0.025707	–3.946152
1	–2.936019	1.513210	–2.397302
1	–1.439991	0.640235	–2.708029
6	–4.606490	–0.225318	–3.841474
1	–6.002557	–1.345613	–2.616498
1	–4.488632	–2.177589	–2.935309
1	–2.889266	0.752757	–4.735726
1	–2.596289	–0.904893	–4.231630
1	–4.994676	–0.612016	–4.788692
1	–5.120688	0.727468	–3.658603
6	–2.300462	1.792603	0.479104
6	–3.755750	2.279463	0.482834
6	–1.576184	2.147780	1.789934
1	–1.785171	2.331284	–0.326259
6	–3.821017	3.778398	0.793516
1	–4.347025	1.726398	1.218385

1	–4.218378	2.097947	–0.490020
6	–1.655927	3.645984	2.075209
1	–2.026549	1.598865	2.624751
1	–0.532274	1.821388	1.745205
6	–3.106533	4.125984	2.098823
1	–4.866521	4.099620	0.832727
1	–3.354601	4.333918	–0.030806
1	–1.161088	3.867078	3.025654
1	–1.103363	4.193875	1.300274
1	–3.149977	5.204806	2.276801
1	–3.629707	3.649299	2.937993
17	1.008967	–1.732938	2.204475
7	2.629077	1.918204	–0.371013
6	3.212937	2.714916	0.716337
6	4.550818	3.356298	0.343819
1	3.385771	2.012283	1.529793
1	5.252125	2.612567	–0.038299
1	5.003849	3.829171	1.220070
1	4.435709	4.131678	–0.419007
1	2.671623	4.237356	2.152165
6	2.239912	3.759274	1.268822
1	1.298130	3.291524	1.563289
1	2.023816	4.548707	0.543015
6	2.143544	2.651440	–1.548621
1	2.694186	3.597339	–1.554133
6	2.510784	1.915454	–2.836236
1	1.981712	0.959740	–2.899657
1	3.584340	1.715584	–2.878040
1	2.234320	2.508381	–3.712931
6	0.651692	3.005248	–1.545051
1	0.044852	2.126945	–1.772959
1	0.330242	3.397597	–0.579986
1	0.443599	3.762031	–2.308203

4–3NTS3

SCF energy = –2354.95557056

7	–3.196835	1.338212	0.580798
15	2.088792	0.368068	–0.106244
6	–2.600155	2.655831	0.867621
1	–3.427166	3.299161	1.178694
6	–2.026620	3.296357	–0.396568
1	–1.198197	2.704182	–0.794398
1	–1.656231	4.305956	–0.189551
1	–2.792354	3.360458	–1.173835
6	–4.573453	1.185754	1.077865
1	–4.873305	0.181789	0.785577
6	–4.638775	1.242112	2.608932
1	–5.652704	1.008022	2.947495
1	–4.392764	2.237818	2.990959
1	–3.953160	0.524676	3.060909
79	–0.311181	0.193937	0.130061
5	–2.443114	0.220630	0.108183
7	–3.049345	–1.027540	–0.432742
6	–3.777641	–1.101710	–1.729985
6	–4.160132	–2.557898	–2.022247
1	–3.295284	–3.211475	–2.127020
1	–4.729324	–2.613134	–2.954688
1	–4.791050	–2.948321	–1.218773
6	–2.927283	–0.517598	–2.874812
1	–1.986785	–1.051420	–2.998239
1	–3.473547	–0.561463	–3.822538
1	–2.694324	0.532691	–2.669844
6	–5.081118	–0.303547	–1.694379
1	–5.596690	–0.410988	–2.652936
1	–5.756030	–0.658783	–0.912274
1	–4.887980	0.755874	–1.544263
5	–1.958685	–1.915593	–0.075304
17	–0.866493	–2.734524	–1.350506
6	–1.883031	–2.642999	1.357542
6	–2.730306	–3.923340	1.178684
1	–2.303401	–4.597376	0.430939
1	–3.755056	–3.687134	0.876127
1	–2.785500	–4.469384	2.127983
6	–0.475859	–3.043243	1.811139
1	0.008505	–3.713196	1.097059
1	–0.518158	–3.560395	2.777153
1	0.163272	–2.164099	1.936352
6	–2.536949	–1.802654	2.459646
1	–2.552107	–2.356363	3.405992
1	–3.568007	–1.549688	2.202595
1	–1.994389	–0.866552	2.627641
6	–5.573973	2.194776	0.494779
1	–6.593219	1.811859	0.598334
1	–5.539737	3.154356	1.019191
1	–5.395722	2.390944	–0.562722
6	–1.595666	2.679542	2.025118
1	–1.383675	3.715389	2.310129
1	–1.990743	2.158046	2.898695
1	–0.648894	2.205090	1.757348
6	2.494287	1.900681	–1.060795
6	2.063674	3.162940	–0.295183
6	2.267893	4.433354	–1.122757
6	1.560788	4.345982	–2.473458

6	2.026088	3.114090	–3.246065
6	1.802493	1.838232	–2.435126
1	3.580353	1.941998	–1.213312
1	2.619990	3.253061	0.642092
1	1.004758	3.076033	–0.023596
1	1.907445	5.297768	–0.556534
1	3.341856	4.592496	–1.286115
1	1.740872	5.255022	–3.055396
1	0.476958	4.283307	–2.312336
1	1.498633	3.037182	–4.201577
1	3.093310	3.215191	–3.483950
1	2.151340	0.972817	–3.005276
1	0.725256	1.690736	–2.286360
6	2.725295	–2.351193	–0.353549
6	2.760203	–1.023382	–1.124125
6	4.118201	–0.827653	–1.812404
1	1.995437	–1.102564	–1.909266
6	3.021554	–3.524895	–1.286122
1	1.751952	–2.487762	0.122162
1	3.477857	–2.333002	0.444062
6	4.361402	–3.342019	–1.999382
1	3.015293	–4.459988	–0.717841
1	2.214769	–3.603852	–2.024593
6	4.416778	–2.006982	–2.743114
1	4.539794	–4.167934	–2.694824
1	5.172015	–3.375685	–1.259231
1	5.396788	–1.870404	–3.211296
1	3.679723	–2.015540	–3.556381
1	4.139916	0.103449	–2.385513
1	4.913377	–0.750619	–1.064433
6	3.009299	0.529034	1.489331
1	2.746167	1.546090	1.809303
6	2.455997	–0.411341	2.572961
1	2.620422	–1.456122	2.290533
1	1.373392	–0.280151	2.657814
6	3.120329	–0.143210	3.924191
1	2.833890	0.857177	4.274256
1	2.742521	–0.852556	4.666674
6	4.643770	–0.228178	3.831921
1	5.097212	–0.003604	4.802180
1	4.933884	–1.257541	3.583258
6	5.185000	0.719313	2.761542
1	4.983540	1.757269	3.056835
1	6.272126	0.622880	2.679093
6	4.537602	0.445217	1.402347
1	4.826493	–0.559151	1.074343
1	4.922304	1.144181	0.652491

4–3NiPr

SCF energy = –711.992916123

7	1.701626	–0.363632	0.023159
7	–0.709808	0.779691	0.062505
6	2.622288	0.772364	–0.019718
1	1.990906	1.661471	–0.043023
6	3.484455	0.866015	1.240518
1	4.165516	0.014862	1.333592
1	2.852628	0.891434	2.131869
1	4.095371	1.773397	1.225039
6	2.293325	–1.712552	0.028710
1	3.380253	–1.587220	0.034792
6	1.916131	–2.485514	1.290521
1	2.414312	–3.459455	1.315061
1	0.836171	–2.651485	1.326097
1	2.204407	–1.928298	2.185764
6	–0.971569	2.219865	0.011665
6	–2.474695	2.477786	0.085481
1	–3.000647	1.961295	–0.720920
1	–2.683135	3.547369	–0.004874
6	–0.421631	2.763300	–1.311311
1	0.649915	2.572639	–1.407118
1	–0.582114	3.842796	–1.383786
1	–0.922941	2.284521	–2.156586
6	–2.638106	–1.282471	0.006984
6	–2.383345	–2.776412	0.268336
6	–3.211312	–1.122084	–1.413455
1	–2.512716	–1.485097	–2.174319
1	–3.440138	–0.077603	–1.644879
1	–4.140336	–1.695651	–1.518671
5	0.311390	–0.226670	0.054351
5	–1.259202	–0.513816	0.070167
1	–3.312420	–3.354062	0.182726
1	–1.662489	–3.187546	–0.444499
6	3.465742	0.792873	–1.295951
1	4.151486	–0.057806	–1.348609
1	2.822066	0.763040	–2.178716
1	4.070488	1.703189	–1.341741
6	1.926621	–2.489186	–1.234246
1	2.416952	–3.467324	–1.249306
1	0.845582	–2.646589	–1.280523
1	2.227910	–1.939168	–2.129492
1	–2.881823	2.132765	1.038198
6	–0.285513	2.893805	1.204243
1	0.795164	2.737956	1.189795

1	–0.471430	3.971632	1.195946
1	–0.670253	2.486536	2.142684
6	–3.664615	–0.772530	1.029700
1	–3.268965	–0.803329	2.050232
1	–3.974739	0.253221	0.822144
1	–4.566363	–1.397080	1.010092
1	–1.978940	–2.941948	1.271938

4

SCF energy = –1634.90504663

79	1.347816	0.276454	0.073090
6	–3.035001	0.402317	–0.304709
17	3.695098	0.095776	–0.156382
6	–0.254156	3.209852	–1.660942
1	–0.092284	4.287498	–1.781274
1	–1.157078	2.947277	–2.217430
1	0.590922	2.699580	–2.134041
15	–0.225892	–2.091797	–1.087694
6	–0.454782	–1.322302	–2.715519
1	–1.464724	–0.928233	–2.817866
1	–0.262487	–2.048181	–3.507848
1	0.248046	–0.492866	–2.809609
7	–1.576913	0.341916	–0.102085
6	–0.662466	–1.349905	1.896870
5	–0.538192	1.251335	–0.061011
5	–0.606625	–0.721237	0.380705
6	–0.353677	2.851468	–0.164855
6	–0.616993	–0.194558	2.913061
1	–0.742794	–0.571486	3.934990
1	–1.408194	0.539064	2.732163
1	0.338783	0.336265	2.872810
6	0.943108	3.333725	0.519065
1	0.974149	3.055246	1.576883
1	1.006756	4.426919	0.465193
1	1.845663	2.939119	0.045242
6	0.528179	–2.281609	2.187507
1	0.535998	–2.571800	3.244390
1	1.494638	–1.817380	1.971474
1	0.466760	–3.214163	1.614088
6	–1.931071	–2.171260	2.191623
1	–1.863903	–2.619693	3.189865
1	–2.074270	–2.996126	1.486243
1	–2.837288	–1.563705	2.182374
6	–3.740535	0.938002	0.947528
1	–3.610898	0.261448	1.793256
1	–4.813913	1.046391	0.766155
1	–3.346488	1.910606	1.238113
6	–3.354124	1.294646	–1.510337
1	–4.423519	1.254173	–1.734406
1	–2.808501	0.957789	–2.395804
1	–3.095890	2.336720	–1.337570
6	–3.591026	–0.987605	–0.627281
1	–3.350964	–1.715359	0.145147
1	–3.214113	–1.353603	–1.585554
1	–4.679489	–0.939409	–0.709640
6	1.441039	–2.816695	–1.197487
1	2.178578	–2.056946	–1.455254
1	1.439075	–3.596848	–1.962576
1	1.731968	–3.251246	–0.241992
6	–1.260601	–3.596913	–1.115957
1	–1.007932	–4.213273	–0.251012
1	–1.057144	–4.171306	–2.022734
1	–2.321717	–3.360350	–1.074028
6	–1.494742	3.646730	0.490886
1	–1.586762	3.408669	1.555128
1	–2.467008	3.484614	0.026850
1	–1.286148	4.720255	0.417464

4–3tI1

SCF energy = –1885.55516871

79	–0.383805	–0.766285	–0.924528
6	1.929111	2.251894	1.290830
17	–1.847937	–2.527248	–1.616854
6	–0.831307	3.781478	–0.844977
1	–1.237597	4.443116	–1.619642
1	0.051777	4.279717	–0.440308
1	–1.581702	3.729245	–0.047256
15	1.311789	–1.546635	1.637789
6	0.158627	–0.876384	2.875039
1	0.411895	0.151559	3.127797
1	0.154013	–1.488247	3.779734
1	–0.837546	–0.882826	2.438915
7	1.258133	1.253122	0.457697
6	2.792215	–0.632431	–0.933921
5	–0.039118	1.321839	–0.262310
5	1.539776	–0.095278	–0.005590
6	–0.510869	2.398198	–1.443542
6	2.780457	0.065536	–2.300457
1	3.640521	–0.255592	–2.901071
1	2.836930	1.149193	–2.195771
1	1.876342	–0.171806	–2.867064
6	–1.787972	1.940187	–2.175628

1	–1.653628	0.982659	–2.687097
1	–2.074722	2.678240	–2.934115
1	–2.642289	1.833904	–1.501280
6	2.753450	–2.147834	–1.196953
1	3.535080	–2.426950	–1.912781
1	1.798661	–2.483339	–1.613222
1	2.949967	–2.732572	–0.292236
6	4.162522	–0.328611	–0.302872
1	4.963307	–0.721748	–0.941212
1	4.290506	–0.787530	0.681724
1	4.337395	0.744385	–0.200042
6	2.725383	3.246644	0.431339
1	3.443333	2.717538	–0.199302
1	3.275960	3.960166	1.052986
1	2.066719	3.815980	–0.224684
6	0.891663	3.017315	2.124625
1	1.381044	3.761773	2.759100
1	0.334424	2.337174	2.775981
1	0.169375	3.541145	1.500336
6	2.897182	1.596179	2.282544
1	3.652239	0.993298	1.781997
1	2.366536	0.965735	2.999067
1	3.418683	2.365253	2.858558
6	0.591202	–3.200696	1.343020
1	–0.385542	–3.111181	0.866276
1	0.486662	–3.731429	2.293110
1	1.227965	–3.782557	0.677525
6	2.786789	–1.988879	2.632128
1	3.470027	–2.582703	2.022768
1	2.493422	–2.580586	3.503146
1	3.313038	–1.096410	2.968238
6	0.564042	2.592134	–2.517081
1	0.718252	1.678352	–3.091891
1	1.525690	2.886992	–2.094951
1	0.257224	3.375061	–3.221813
6	–1.370671	1.106696	0.643177
7	–2.409984	0.935483	1.134013
6	–3.710039	0.324869	1.383016
6	–4.486547	1.226609	2.339558
1	–5.468807	0.790101	2.532584
1	–3.963751	1.333307	3.292758
1	–4.630193	2.219385	1.907942
6	–3.472826	–1.061975	1.983311
1	–2.875480	–1.679365	1.307663
1	–2.981359	–0.994416	2.956485
1	–4.436750	–1.554731	2.126554
6	–4.409421	0.202327	0.026710
1	–5.381081	–0.275382	0.171308
1	–4.574209	1.184115	–0.421290
1	–3.821941	–0.411376	–0.659815

4–3tI2

SCF energy = –1424.45269449

79	0.326569	–1.160248	0.197226
6	–2.192848	2.263512	–0.891900
17	1.991283	–2.833276	0.160312
6	–0.384204	2.799906	2.423469
1	–0.345685	2.999001	3.500842
1	–1.288437	3.280959	2.045255
1	0.477620	3.307286	1.974232
7	–1.500169	1.071219	–0.379704
6	–2.609210	–1.474402	–0.752638
5	–0.322958	0.931180	0.561212
5	–1.564760	–0.297811	–0.428346
6	–0.360941	1.284926	2.158143
6	–2.898777	–2.193950	0.583314
1	–3.601725	–3.017745	0.415357
1	–3.348773	–1.517733	1.316455
1	–1.996343	–2.618694	1.031696
6	0.876906	0.727874	2.884874
1	0.948725	–0.360923	2.809700
1	0.841439	0.980155	3.951058
1	1.810176	1.144389	2.488106
6	–2.029249	–2.493463	–1.752017
1	–2.776502	–3.264280	–1.973675
1	–1.140897	–3.000972	–1.367292
1	–1.755203	–2.017932	–2.698932
6	–3.955849	–0.991087	–1.309875
1	–4.671578	–1.821114	–1.314631
1	–3.868185	–0.645519	–2.341556
1	–4.394792	–0.189440	–0.710371
6	–3.367081	2.644090	0.014752
1	–4.079151	1.819788	0.091678
1	–3.895486	3.513010	–0.387864
1	–3.031381	2.891524	1.022577
6	–1.189564	3.419357	–0.974527
1	–1.688007	4.323748	–1.331748
1	–0.386601	3.181852	–1.678425
1	–0.739850	3.649082	–0.008814
6	–2.702446	1.999910	–2.311634
1	–3.529858	1.295635	–2.320259
1	–1.901211	1.602245	–2.940156
1	–3.058024	2.931428	–2.760153

6	–1.610404	0.652672	2.786261
1	–1.582197	–0.438160	2.706936
1	–2.530185	0.992424	2.301805
1	–1.683199	0.904988	3.850605
6	1.069610	1.331275	–0.094915
7	2.123654	1.561439	–0.518542
6	3.470257	1.261833	–0.992799
6	4.134755	2.570967	–1.409232
1	5.150610	2.368010	–1.754237
1	3.585796	3.049057	–2.223656
1	4.189930	3.267691	–0.569974
6	3.323294	0.295382	–2.170255
1	2.838623	–0.631314	–1.856006
1	2.744109	0.747760	–2.978516
1	4.315898	0.049891	–2.554174
6	4.199915	0.595453	0.176488
1	5.218444	0.349935	–0.132157
1	4.253084	1.266471	1.036893
1	3.697241	–0.328187	0.471550

4–3tI3

SCF energy = –1885.56691773

79	–0.805926	–0.191904	0.277379
6	2.296803	2.220684	–1.289357
17	–0.695364	–2.693322	1.260735
6	3.209870	0.529481	2.449076
1	3.453476	0.692354	3.505905
1	3.890698	1.150752	1.864712
1	3.441968	–0.519118	2.229990
15	–2.995358	–0.995581	–0.475153
6	–2.904765	–2.540393	–1.437020
1	–2.362828	–2.358630	–2.367684
1	–3.905481	–2.913866	–1.670134
1	–2.358507	–3.277738	–0.848951
7	1.240198	1.713791	–0.408836
6	–1.248362	2.950100	–0.353443
5	1.263850	0.581609	0.627376
5	–0.124603	1.801125	–0.235336
6	1.727162	0.847106	2.185383
6	–0.711051	4.355948	–0.028447
1	–1.544866	5.064003	0.046926
1	–0.039390	4.740574	–0.791529
1	–0.178223	4.375003	0.926352
6	0.909927	–0.020762	3.156645
1	–0.158525	0.209951	3.102705
1	1.235144	0.150305	4.191066
1	1.007821	–1.088737	2.945718
6	–2.395410	2.703588	0.643880
1	–3.155103	3.489120	0.551735
1	–2.032333	2.714104	1.676253
1	–2.890446	1.744643	0.489966
6	–1.808079	2.937603	–1.785456
1	–2.629233	3.657722	–1.889198
1	–2.193331	1.951588	–2.056945
1	–1.043346	3.204504	–2.521617
6	2.109927	3.694812	–1.636264
1	1.175180	3.858207	–2.175251
1	2.925136	4.031494	–2.282768
1	2.110226	4.311955	–0.735980
6	3.668516	2.043405	–0.640815
1	4.451612	2.379186	–1.325498
1	3.868182	0.997527	–0.397475
1	3.745678	2.630321	0.276414
6	2.241970	1.397954	–2.588671
1	1.263879	1.509323	–3.064646
1	2.398448	0.335347	–2.386951
1	3.010416	1.725237	–3.295896
6	–4.047941	–1.423514	0.946307
1	–3.487635	–2.110343	1.582484
1	–4.984298	–1.886774	0.624654
1	–4.268605	–0.519528	1.518071
6	–4.100002	0.022539	–1.518504
1	–4.288764	0.991047	–1.054271
1	–5.053975	–0.487475	–1.676656
1	–3.630119	0.195839	–2.488478
6	1.468408	2.317562	2.535715
1	0.408481	2.569550	2.416915
1	2.037598	3.003687	1.900957
1	1.737078	2.520740	3.579208
6	1.846892	–0.756975	0.042418
7	2.289364	–1.730977	–0.395799
6	2.504638	–3.044580	–0.963350
6	1.278716	–3.363981	–1.823661
1	1.402165	–4.352367	–2.272816
1	0.378566	–3.360555	–1.206739
1	1.168018	–2.629707	–2.626135
6	2.637121	–4.027748	0.201145
1	3.493949	–3.772437	0.829121
1	1.731568	–4.017655	0.809953
1	2.788991	–5.032990	–0.199241
6	3.781919	–2.985200	–1.802034
1	3.963806	–3.962521	–2.254082
1	3.691586	–2.247417	–2.602995

1	4.644319	–2.724791	–1.184368

4–3tI4

SCF energy = –1885.55696543

79	0.657523	–0.423655	0.051713
6	–3.724108	0.368888	–0.502966
17	1.087781	–2.698830	1.592347
6	–2.004408	1.883982	2.920694
1	–1.883669	1.917386	4.009681
1	–3.074514	1.905866	2.724304
1	–1.575430	2.812575	2.524820
15	3.057159	–0.546826	–0.217663
6	3.965065	0.598577	–1.316578
1	3.569339	0.516802	–2.330928
1	5.030571	0.355195	–1.332812
1	3.844554	1.630104	–0.984456
7	–2.340792	–0.016401	–0.177071
6	–1.359995	–2.242624	–1.507215
5	–1.284880	0.606906	0.712044
5	–1.398381	–0.898093	–0.619982
6	–1.295306	0.636802	2.355260
6	–1.948629	–3.356017	–0.616138
1	–1.967516	–4.302262	–1.170547
1	–2.970249	–3.135785	–0.297793
1	–1.335755	–3.504235	0.276456
6	0.130464	0.677655	2.944401
1	0.686463	–0.241256	2.747672
1	0.082235	0.792893	4.033869
1	0.707018	1.530084	2.560581
6	0.042188	–2.698834	–1.954498
1	–0.048739	–3.600613	–2.571797
1	0.676399	–2.953961	–1.104160
1	0.544049	–1.937954	–2.563416
6	–2.192929	–2.098971	–2.793277
1	–2.146258	–3.036133	–3.359726
1	–1.802846	–1.308086	–3.442640
1	–3.246795	–1.893955	–2.609591
6	–4.656784	–0.839975	–0.395497
1	–4.423123	–1.611427	–1.126980
1	–5.694003	–0.532666	–0.556417
1	–4.581473	–1.287292	0.598458
6	–4.225333	1.433868	0.468418
1	–5.201722	1.800011	0.141497
1	–3.546664	2.289046	0.515187
1	–4.342343	1.023684	1.471566
6	–3.744073	0.968449	–1.915761
1	–3.375815	0.262338	–2.658916
1	–3.111131	1.860257	–1.953221
1	–4.759924	1.261791	–2.196682
6	3.919122	–0.396153	1.375500
1	3.746149	0.595553	1.798822
1	4.993535	–0.561274	1.262444
1	3.494753	–1.141316	2.050862
6	3.565857	–2.172803	–0.853022
1	3.164548	–2.935370	–0.184068
1	4.655073	–2.247849	–0.904261
1	3.143051	–2.325037	–1.848015
6	–1.992846	–0.629631	2.866341
1	–1.457245	–1.529009	2.549414
1	–3.021512	–0.701598	2.498080
1	–2.031748	–0.635692	3.962168
6	–0.665673	1.891497	0.089303
7	–0.266960	2.924983	–0.298654
6	0.879753	3.612785	–0.888561
6	1.238618	2.878733	–2.181043
1	2.136848	3.319979	–2.619939
1	1.423376	1.821046	–1.984154
1	0.426750	2.955404	–2.907770
6	2.008352	3.524962	0.142239
1	1.732777	4.040420	1.064625
1	2.219373	2.481547	0.385348
1	2.913306	3.990063	–0.256522
6	0.491839	5.062954	–1.160498
1	1.341272	5.598223	–1.591319
1	–0.340890	5.117206	–1.865003
1	0.197466	5.567528	–0.237831

4–3tI5

SCF energy = –1885.55704187

79	0.981704	–0.068928	0.225516
6	–3.436014	–1.047857	0.172622
17	–0.191467	–3.038172	–0.009341
6	–2.307392	0.862495	3.189139
1	–2.174090	0.958860	4.274507
1	–3.192205	0.246981	3.034885
1	–2.533055	1.863283	2.802705
15	3.316483	–0.458640	0.150893
6	4.386683	0.828167	–0.573103
1	4.101410	0.987720	–1.614722
1	5.441833	0.545567	–0.529294
1	4.243429	1.766743	–0.034618
7	–1.991533	–0.805822	0.083945

6	–0.709734	–1.300740	–2.326875
5	–1.162471	0.180637	0.880851
5	–0.978370	–1.420885	–0.709773
6	–1.033164	0.288069	2.540419
6	–1.386291	–2.461095	–3.090713
1	–1.112254	–2.409097	–4.151715
1	–2.472468	–2.432256	–3.044678
1	–1.057402	–3.431547	–2.710737
6	0.092841	1.250685	2.975000
1	1.087475	0.871881	2.717088
1	0.076595	1.395700	4.062653
1	–0.010991	2.241541	2.516943
6	0.777396	–1.377594	–2.721799
1	0.876222	–1.413982	–3.813699
1	1.250943	–2.273329	–2.313900
1	1.339780	–0.502624	–2.379532
6	–1.256946	0.033772	–2.849160
1	–1.145811	0.105031	–3.938423
1	–0.710626	0.871512	–2.406884
1	–2.312065	0.176682	–2.606651
6	–3.940834	–1.804565	–1.057095
1	–3.801483	–1.228063	–1.972527
1	–5.010606	–2.006027	–0.953998
1	–3.433572	–2.766651	–1.160968
6	–3.775693	–1.932449	1.385157
1	–4.847424	–2.155959	1.418209
1	–3.507531	–1.462660	2.328287
1	–3.228107	–2.875996	1.316850
6	–4.188190	0.285913	0.239903
1	–4.005348	0.867072	–0.669056
1	–3.876638	0.893818	1.089438
1	–5.265934	0.119021	0.328868
6	4.019097	–0.715339	1.812417
1	3.856493	0.177782	2.418593
1	5.089381	–0.932663	1.767124
1	3.500107	–1.547652	2.291471
6	3.787873	–1.965838	–0.752527
1	3.188604	–2.801487	–0.386743
1	4.851086	–2.186651	–0.628111
1	3.566214	–1.834100	–1.812434
6	–0.729000	–1.089298	3.145419
1	0.250533	–1.455251	2.820595
1	–1.452674	–1.845274	2.839506
1	–0.724185	–1.043836	4.242743
6	–1.187444	1.589210	0.245156
7	–1.233156	2.669379	–0.221321
6	–0.559089	3.718518	–0.968772
6	0.881449	3.292308	–1.259246
1	1.396881	4.085123	–1.807300
1	1.422230	3.100210	–0.328949
1	0.909581	2.379825	–1.859178
6	–0.587927	4.976354	–0.098440
1	–1.616538	5.263309	0.129264
1	–0.061437	4.807279	0.843775
1	–0.103799	5.804239	–0.622267
6	–1.340993	3.938296	–2.264885
1	–0.882989	4.747671	–2.838732
1	–1.342534	3.035580	–2.878841
1	–2.376709	4.208759	–2.049350

4–3tI6

SCF energy = –1885.55766480

79	–0.983233	–0.685438	0.009920
6	2.757629	1.898153	–0.159326
17	–0.925651	2.458501	1.430684
6	2.392322	–1.367866	2.713841
1	2.449722	–1.631520	3.777572
1	3.379851	–1.001441	2.420866
1	2.197843	–2.290988	2.157968
15	–3.294063	–0.781601	–0.091323
6	–3.978029	–2.398764	0.391389
1	–3.608656	–3.167199	–0.289597
1	–5.070721	–2.389690	0.370573
1	–3.637635	–2.644148	1.398845
7	1.406162	1.449001	0.277185
6	–0.435939	2.648755	–1.431920
5	1.218122	0.051805	0.865181
5	0.183460	2.101196	–0.027448
6	1.287180	–0.322198	2.472139
6	0.204487	3.973300	–1.895886
1	–0.339644	4.354336	–2.767908
1	1.246605	3.866723	–2.196362
1	0.152001	4.742355	–1.119100
6	–0.017011	–0.934633	3.019860
1	–0.858678	–0.242356	2.921915
1	0.093975	–1.168737	4.086787
1	–0.275160	–1.870368	2.511631
6	–1.946951	2.931471	–1.332276
1	–2.344556	3.164721	–2.327445
1	–2.172386	3.771502	–0.672936
1	–2.489923	2.063568	–0.951825
6	–0.272617	1.589008	–2.543673
1	–0.495427	2.031613	–3.522119

1	–0.969993	0.757768	–2.398023
1	0.722335	1.153218	–2.589760
6	2.906684	3.387834	0.175298
1	2.180996	4.009424	–0.347087
1	3.904800	3.745863	–0.095737
1	2.763861	3.540580	1.247708
6	3.844322	1.165507	0.635986
1	4.829609	1.475394	0.278450
1	3.774734	0.087322	0.521177
1	3.791769	1.400075	1.697559
6	3.035245	1.638777	–1.647143
1	2.433458	2.268129	–2.300138
1	2.824516	0.595295	–1.894382
1	4.085446	1.836906	–1.881182
6	–4.105497	0.386547	1.039783
1	–3.768986	0.183898	2.057984
1	–5.193256	0.294450	0.987745
1	–3.808010	1.406428	0.793176
6	–4.053443	–0.459109	–1.713673
1	–3.772951	0.536955	–2.059282
1	–5.142830	–0.528959	–1.659688
1	–3.679995	–1.187200	–2.435908
6	1.587516	0.907163	3.344037
1	0.823765	1.676570	3.235395
1	2.548032	1.367924	3.111780
1	1.623054	0.615056	4.401344
6	1.171148	–1.078450	–0.123117
7	1.247286	–2.055254	–0.887699
6	2.473090	–2.759349	–1.301876
6	3.772198	–2.177353	–0.752615
1	4.616509	–2.806132	–1.049406
1	3.954569	–1.175202	–1.142844
1	3.756095	–2.129129	0.337769
6	2.487355	–2.718684	–2.831856
1	1.565374	–3.143208	–3.235318
1	2.570559	–1.688125	–3.188750
1	3.335788	–3.286097	–3.225350
6	2.301938	–4.201663	–0.815703
1	3.129667	–4.826968	–1.162794
1	2.278357	–4.238959	0.276988
1	1.366167	–4.622487	–1.190400

4–3tTS1

SCF energy = –1885.54935401

79	–0.399260	–0.628743	–0.953762
6	2.193587	2.025142	1.386767
17	–2.053176	–2.143177	–1.792931
6	–0.439171	3.884701	–0.574663
1	–0.840681	4.612744	–1.289628
1	0.506504	4.292307	–0.212806
1	–1.136580	3.843194	0.268588
15	1.155212	–1.670133	1.557375
6	0.062653	–0.964398	2.826259
1	0.401357	0.027034	3.121635
1	0.018331	–1.616793	3.700902
1	–0.933936	–0.868506	2.400692
7	1.400204	1.133480	0.532471
6	2.770276	–0.827623	–0.927300
5	0.214329	1.328246	–0.236018
5	1.548908	–0.258885	0.030600
6	–0.276505	2.517528	–1.259958
6	2.814489	–0.033892	–2.240768
1	3.649021	–0.372569	–2.867283
1	2.949839	1.033464	–2.060002
1	1.895293	–0.161921	–2.817817
6	–1.623952	2.216067	–1.946653
1	–1.605189	1.285476	–2.520785
1	–1.873521	3.021594	–2.647140
1	–2.449197	2.147931	–1.234016
6	2.592348	–2.310831	–1.299679
1	3.336783	–2.605223	–2.048362
1	1.605898	–2.524294	–1.722159
1	2.745173	–2.978471	–0.444702
6	4.168831	–0.697106	–0.297628
1	4.921792	–1.130703	–0.967130
1	4.260868	–1.219314	0.658960
1	4.452033	0.345558	–0.140285
6	3.083620	2.949171	0.544129
1	3.740456	2.367967	–0.106679
1	3.707802	3.585319	1.179573
1	2.482208	3.600441	–0.090417
6	1.260028	2.867535	2.266261
1	1.843949	3.515677	2.926294
1	0.631846	2.227238	2.891780
1	0.597839	3.499677	1.679968
6	3.083866	1.223043	2.341733
1	3.755775	0.550335	1.813810
1	2.482996	0.638677	3.042281
1	3.697979	1.902263	2.938508
6	0.293319	–3.227885	1.151866
1	–0.684200	–3.023465	0.714227
1	0.168050	–3.819928	2.062340
1	0.864743	–3.804867	0.426189

6	2.578325	–2.307940	2.516192
1	3.203122	–2.927993	1.871813
1	2.222032	–2.921041	3.347850
1	3.188085	–1.495584	2.908652
6	0.758404	2.680080	–2.385835
1	0.819387	1.784445	–3.006264
1	1.759330	2.890041	–2.005359
1	0.471227	3.512312	–3.039615
6	–1.472858	1.273148	0.942085
7	–2.546224	0.923398	1.216431
6	–3.859282	0.317345	1.320088
6	–4.636669	1.049618	2.413096
1	–5.630392	0.606902	2.509964
1	–4.128803	0.967845	3.376838
1	–4.753138	2.107787	2.169587
6	–3.660649	–1.160316	1.665881
1	–3.065993	–1.659026	0.897276
1	–3.178952	–1.276055	2.640104
1	–4.635282	–1.651004	1.710923
6	–4.529104	0.463610	–0.048466
1	–5.517350	–0.000590	–0.013646
1	–4.651726	1.516212	–0.312682
1	–3.940776	–0.035299	–0.821266

4–3tTS2

SCF energy = –1885.55454612

79	–0.371230	–0.626759	–1.031911
6	1.943394	2.111137	1.511012
17	–1.853798	–2.292358	–1.878953
6	–0.796998	3.901818	–0.427475
1	–1.186711	4.653328	–1.124612
1	0.099579	4.329604	0.025051
1	–1.546721	3.781730	0.363702
15	1.273882	–1.825148	1.533774
6	0.144640	–1.273505	2.861622
1	0.492403	–0.342934	3.309845
1	0.042976	–2.032654	3.641581
1	–0.832559	–1.088599	2.420152
7	1.265527	1.237465	0.548354
6	2.793570	–0.515576	–1.015749
5	–0.056176	1.377450	–0.132264
5	1.528626	0.019938	–0.129889
6	–0.516333	2.583381	–1.172551
6	2.850573	0.300752	–2.319077
1	3.716429	–0.005743	–2.918209
1	2.946839	1.370072	–2.123595
1	1.957592	0.148785	–2.930572
6	–1.809010	2.236404	–1.935778
1	–1.708193	1.328827	–2.537452
1	–2.077117	3.051926	–2.617829
1	–2.661710	2.092481	–1.265660
6	2.697479	–1.998712	–1.409940
1	3.497062	–2.251458	–2.115643
1	1.748400	–2.253104	–1.890487
1	2.823424	–2.663391	–0.550289
6	4.148189	–0.329271	–0.314457
1	4.953448	–0.711072	–0.953607
1	4.206825	–0.873253	0.632524
1	4.369415	0.722522	–0.119344
6	2.753409	3.198133	0.791674
1	3.480460	2.747258	0.111980
1	3.296591	3.825051	1.505788
1	2.107518	3.847940	0.200678
6	0.900252	2.759811	2.430290
1	1.387696	3.402637	3.168346
1	0.335402	1.995330	2.972595
1	0.188446	3.372515	1.879083
6	2.888825	1.311220	2.413822
1	3.660643	0.791986	1.851682
1	2.339454	0.576107	3.003761
1	3.387091	1.984151	3.116850
6	0.497219	–3.421125	1.078509
1	–0.475178	–3.247434	0.614108
1	0.371835	–4.061064	1.956653
1	1.114726	–3.941620	0.345109
6	2.725643	–2.413356	2.493827
1	3.420737	–2.924768	1.824552
1	2.425565	–3.109066	3.282543
1	3.250843	–1.569903	2.944736
6	0.567903	2.849942	–2.220711
1	0.692317	1.993845	–2.885951
1	1.537658	3.061061	–1.767193
1	0.295334	3.712503	–2.841386
6	–1.361706	1.032412	0.751460
7	–2.393289	0.792864	1.227651
6	–3.691495	0.152896	1.408124
6	–4.412560	0.852205	2.557614
1	–5.390983	0.390395	2.706224
1	–3.847016	0.763565	3.487969
1	–4.561812	1.911986	2.340392
6	–3.452961	–1.328270	1.707803
1	–2.871523	–1.798740	0.911288
1	–2.947136	–1.464477	2.665820

1	–4.419047	–1.834368	1.764050
6	–4.443187	0.313366	0.084091
1	–5.420383	–0.166733	0.171992
1	–4.599334	1.367571	–0.153563
1	–3.896762	–0.162764	–0.733008

4–3tTS3

SCF energy = –1885.55262781

79	–0.449696	–0.089233	–0.848106
6	2.850375	–0.865772	1.811327
17	–2.266175	1.222694	–1.811230
6	3.496270	2.149317	–1.042926
1	4.120391	2.457158	–1.889882
1	4.170783	1.920031	–0.217400
1	2.904962	3.025495	–0.753247
15	–3.035350	–1.174621	0.770302
6	–4.077196	0.185802	1.434300
1	–3.630003	0.598984	2.341438
1	–5.091804	–0.154450	1.662332
1	–4.129764	0.976015	0.682656
7	1.939980	–0.725377	0.665320
6	0.635519	–3.015820	–0.147022
5	1.626598	0.452554	–0.224699
5	0.937811	–1.444309	0.039872
6	2.598982	0.963502	–1.447303
6	1.856025	–3.663299	–0.830301
1	1.690420	–4.740928	–0.948773
1	2.783709	–3.527489	–0.276692
1	2.009197	–3.247640	–1.830879
6	1.781710	1.437242	–2.662981
1	1.201658	0.624510	–3.107506
1	2.447882	1.834174	–3.438999
1	1.072018	2.230006	–2.403255
6	–0.572644	–3.308839	–1.051668
1	–0.677508	–4.389831	–1.203940
1	–0.470299	–2.847358	–2.038607
1	–1.502662	–2.948959	–0.610772
6	0.362754	–3.683065	1.210882
1	0.104739	–4.739592	1.068885
1	–0.477431	–3.204127	1.723440
1	1.221743	–3.649927	1.882957
6	3.711241	–2.128125	1.728531
1	3.117455	–3.038948	1.791263
1	4.426978	–2.145381	2.555306
1	4.275093	–2.149204	0.792925
6	3.793321	0.334847	1.889235
1	4.369516	0.293411	2.816890
1	3.249865	1.283065	1.881500
1	4.501211	0.334107	1.059101
6	1.986393	–0.892564	3.081040
1	1.271959	–1.717188	3.050714
1	1.418409	0.038179	3.170555
1	2.604274	–1.003740	3.977250
6	–4.123445	–1.746549	–0.594805
1	–4.123495	–0.986149	–1.377912
1	–5.148679	–1.918589	–0.253237
1	–3.735452	–2.672732	–1.024624
6	–3.359199	–2.490369	2.019782
1	–2.935308	–3.435238	1.670382
1	–4.428696	–2.634190	2.201222
1	–2.872145	–2.235980	2.964509
6	3.485154	–0.205569	–1.891691
1	2.881149	–1.053492	–2.228999
1	4.127716	–0.567035	–1.083422
1	4.132539	0.092127	–2.724981
6	0.940897	1.687592	0.499812
7	0.458625	2.641804	0.945061
6	–0.538769	3.666722	1.210461
6	–1.800718	2.939552	1.676030
1	–2.588842	3.671230	1.867865
1	–2.145349	2.251358	0.903114
1	–1.613186	2.382139	2.597031
6	–0.778726	4.388055	–0.118462
1	0.139698	4.856742	–0.479482
1	–1.147554	3.689376	–0.872330
1	–1.529276	5.167788	0.030217
6	0.010776	4.607834	2.279402
1	–0.726362	5.386083	2.487462
1	0.214793	4.072060	3.209301
1	0.932248	5.087895	1.943020

4–3tTS4

SCF energy = –1885.54870052

79	–0.937561	–0.017791	0.044350
6	3.126122	1.797507	0.296993
17	–1.209182	2.827849	–0.238760
6	2.116835	–0.156272	3.383008
1	1.901772	–0.200139	4.457779
1	2.868009	0.620318	3.244885
1	2.580770	–1.111675	3.109885
15	–3.306353	–0.206528	0.119005
6	–4.126319	–1.826078	0.284605

1	–3.877766	–2.448558	–0.577197
1	–5.212278	–1.720683	0.351192
1	–3.758586	–2.324302	1.183674
7	1.809823	1.165521	0.137493
6	0.679120	1.084416	–2.424122
5	1.125206	0.089375	0.962476
5	0.814327	1.077214	–0.808327
6	0.819375	0.089991	2.586873
6	0.923540	2.462570	–3.063601
1	0.723161	2.404258	–4.140562
1	1.946942	2.812827	–2.951238
1	0.252633	3.207953	–2.632374
6	–0.124150	–1.059127	3.002759
1	–1.137766	–0.923989	2.615728
1	–0.198919	–1.113521	4.095708
1	0.231407	–2.036737	2.656007
6	–0.690686	0.616022	–2.951801
1	–0.674935	0.602776	–4.048412
1	–1.483485	1.295604	–2.635241
1	–0.943229	–0.398819	–2.622931
6	1.722434	0.069118	–2.934334
1	1.691983	0.008501	–4.028666
1	1.515661	–0.933429	–2.544664
1	2.743488	0.324243	–2.643628
6	3.502619	2.608928	–0.939695
1	3.592938	1.985822	–1.829566
1	4.468945	3.093802	–0.778480
1	2.762559	3.388840	–1.124769
6	3.092393	2.786175	1.469889
1	4.048114	3.313011	1.549452
1	2.905632	2.298023	2.423057
1	2.301800	3.522679	1.308480
6	4.181942	0.709963	0.518920
1	4.231750	0.044998	–0.348982
1	3.960085	0.100419	1.396842
1	5.169539	1.156378	0.664117
6	–3.927881	0.769468	1.520506
1	–3.570372	0.337766	2.457414
1	–5.019979	0.811410	1.530734
1	–3.514709	1.776179	1.425153
6	–4.088809	0.564726	–1.327900
1	–3.688068	1.576996	–1.416146
1	–5.175752	0.601301	–1.219611
1	–3.828676	0.010211	–2.231470
6	0.177189	1.408835	3.037920
1	–0.802907	1.554485	2.576160
1	0.769280	2.280322	2.759405
1	0.046545	1.420952	4.127864
6	1.546876	–1.344513	0.479853
7	1.825167	–2.411350	0.096306
6	1.527267	–3.635571	–0.629993
6	0.148082	–3.480359	–1.272560
1	–0.109931	–4.396623	–1.809062
1	–0.614229	–3.287276	–0.514340
1	0.133694	–2.647485	–1.978549
6	1.537483	–4.777552	0.386849
1	2.511548	–4.857995	0.873611
1	0.777411	–4.619779	1.155338
1	1.325328	–5.721766	–0.119866
6	2.617580	–3.828341	–1.683846
1	2.428892	–4.750036	–2.238986
1	2.630420	–2.996739	–2.390989
1	3.601366	–3.902106	–1.215833

4–3tTS5

SCF energy = –1885.55569974

79	1.031121	0.158996	0.208016
6	–3.529456	–0.473696	0.042238
17	–0.432902	–2.906188	0.634818
6	–2.236796	1.576781	3.014729
1	–2.173010	1.763464	4.094300
1	–3.246908	1.219318	2.816266
1	–2.128646	2.539928	2.505314
15	3.191032	–0.779376	0.198611
6	4.113107	–0.623542	–1.364559
1	3.548357	–1.101466	–2.166877
1	5.098175	–1.091577	–1.291260
1	4.232413	0.432700	–1.612339
7	–2.061294	–0.669476	0.196324
6	–0.984126	–1.912604	–2.043051
5	–1.236470	0.377660	0.950893
5	–1.277389	–1.648610	–0.464056
6	–1.127483	0.596224	2.574493
6	–1.811848	–3.074581	–2.633480
1	–1.422135	–3.334420	–3.624758
1	–2.866219	–2.837709	–2.760661
1	–1.739012	–3.970179	–2.008940
6	0.186026	1.271393	3.015549
1	1.054084	0.618630	2.872598
1	0.144730	1.515848	4.084508

1	0.373112	2.205647	2.475201
6	0.489322	–2.317905	–2.274409
1	0.677661	–2.404733	–3.350830
1	0.727472	–3.278717	–1.814874
1	1.182453	–1.568256	–1.883222
6	–1.203229	–0.621947	–2.851460
1	–1.041889	–0.803423	–3.920715
1	–0.496409	0.150448	–2.534145
1	–2.199355	–0.197130	–2.732705
6	–4.120395	–1.344694	–1.067480
1	–3.791379	–1.048035	–2.061160
1	–5.209305	–1.255169	–1.048851
1	–3.881307	–2.399891	–0.910570
6	–4.226421	–0.942745	1.331959
1	–5.311782	–0.829549	1.244045
1	–3.905521	–0.383040	2.205472
1	–4.003916	–1.997606	1.514081
6	–3.873532	0.989138	–0.250354
1	–3.404583	1.321035	–1.179131
1	–3.531883	1.660660	0.538502
1	–4.956795	1.107708	–0.347475
6	4.322417	–0.075781	1.440981
1	4.448974	0.992620	1.257407
1	5.298776	–0.566056	1.412977
1	3.885544	–0.199341	2.433569
6	3.209593	–2.561847	0.548587
1	2.743080	–2.740497	1.518397
1	4.229437	–2.955127	0.549231
1	2.611168	–3.081037	–0.200646
6	–1.243893	–0.722979	3.346277
1	–0.380453	–1.364325	3.149233
1	–2.127206	–1.297781	3.064788
1	–1.288817	–0.539568	4.427799
6	–0.799508	1.523158	0.092480
7	–0.901701	2.596281	–0.499779
6	–0.016696	3.352549	–1.383657
6	1.369205	2.748107	–1.625633
1	1.936103	3.392996	–2.303352
1	1.934109	2.665513	–0.692527
1	1.303094	1.758265	–2.086047
6	0.137189	4.734489	–0.740283
1	–0.841941	5.187482	–0.572805
1	0.642116	4.651763	0.226236
1	0.725188	5.396828	–1.382125
6	–0.762151	3.473555	–2.717462
1	–0.204657	4.106085	–3.414254
1	–0.895414	2.489636	–3.174993
1	–1.749923	3.911899	–2.561728

4–3tTS6

SCF energy = –1885.56163103

79	1.802827	0.129752	0.106569
6	–2.605593	–2.223259	–0.947935
17	–1.694758	1.014218	–2.280297
6	–0.316613	–1.027147	3.113065
1	–0.092929	–1.604012	4.018342
1	–1.169542	–0.377592	3.334461
1	0.541050	–0.380111	2.915064
15	3.911987	–0.275431	–0.783007
6	5.326629	0.265251	0.228822
1	5.251242	1.339219	0.407969
1	6.277631	0.046897	–0.263353
1	5.294828	–0.241396	1.194914
7	–2.024243	–1.003320	–0.297678
6	–3.869445	1.032944	–0.323988
5	–1.000840	–1.004268	0.687629
5	–2.445712	0.377897	–0.717222
6	–0.617219	–1.987564	1.933027
6	–5.017637	0.521110	–1.223254
1	–5.943675	1.038648	–0.948263
1	–5.215588	–0.544611	–1.128215
1	–4.827458	0.738837	–2.278495
6	0.657813	–2.820888	1.701610
1	0.548052	–3.557722	0.902314
1	0.918622	–3.366211	2.617645
1	1.513503	–2.187619	1.447347
6	–3.898366	2.556823	–0.514640
1	–4.876782	2.950789	–0.215416
1	–3.735040	2.834124	–1.558951
1	–3.148710	3.061974	0.083337
6	–4.194400	0.702607	1.141123
1	–5.145455	1.159347	1.439834
1	–3.412170	1.078247	1.805646
1	–4.276526	–0.374729	1.306329
6	–1.528287	–3.315079	–1.011752
1	–0.617137	–2.919041	–1.468763
1	–1.880926	–4.150570	–1.622570
1	–1.276840	–3.713922	–0.033722
6	–3.840454	–2.768633	–0.217743
1	–4.162357	–3.707324	–0.679174
1	–4.679439	–2.077371	–0.265501
1	–3.638220	–2.962561	0.831635
6	–2.979575	–1.949693	–2.414037

1	–2.100399	–1.679360	–2.999962
1	–3.715130	–1.158208	–2.535139
1	–3.408685	–2.860050	–2.841916
6	4.261143	–2.032534	–1.108641
1	4.196553	–2.592334	–0.173891
1	5.252592	–2.170892	–1.547204
1	3.505889	–2.426878	–1.790714
6	4.195883	0.528839	–2.391209
1	3.438886	0.190026	–3.100519
1	5.189928	0.302779	–2.785072
1	4.088271	1.608825	–2.276871
6	–1.722820	–2.921516	2.449084
1	–1.952414	–3.746936	1.774679
1	–2.650091	–2.375292	2.644027
1	–1.409560	–3.373641	3.397839
6	–0.174377	0.345636	0.647295
7	–0.933671	1.380507	0.704886
6	–0.419994	2.765911	0.912993
6	–1.340517	3.387083	1.975133
1	–1.109341	4.446961	2.117889
1	–2.394056	3.300448	1.719717
1	–1.196537	2.876427	2.932084
6	–0.438029	3.556576	–0.397113
1	0.222445	3.081653	–1.127613
1	–1.428398	3.616082	–0.843092
1	–0.079517	4.575736	–0.220858
6	0.999959	2.845825	1.492171
1	1.177369	3.865763	1.845332
1	1.128505	2.167381	2.339800
1	1.774852	2.625388	0.753758

4–5tAuMe

SCF energy = –1885.59000775

79	–1.889948	–0.139463	0.029397
6	3.312706	1.819841	–0.921667
17	3.076972	–1.495701	–1.780816
6	–0.387791	2.222975	1.989518
1	–0.891732	3.105660	2.401989
1	0.338705	1.884328	2.735804
1	–1.141082	1.437412	1.893621
15	–4.181696	0.097338	–0.176408
6	–5.153321	–0.421919	1.272557
1	–4.979999	–1.482114	1.464866
1	–6.221378	–0.253134	1.114923
1	–4.824208	0.139653	2.148459
7	2.328200	0.862601	–0.312567
6	3.448447	–1.092301	1.202399
5	1.050007	1.215397	0.145340
5	2.514382	–0.678039	–0.130468
6	0.309813	2.583100	0.654218
6	4.406039	–2.274960	0.977710
1	4.944557	–2.503135	1.906468
1	5.151226	–2.029459	0.216338
1	3.915844	–3.190079	0.652560
6	–0.758577	3.038038	–0.364110
1	–0.303885	3.471160	–1.259125
1	–1.400956	3.808674	0.081521
1	–1.410582	2.226672	–0.698776
6	2.537689	–1.384180	2.411758
1	3.137804	–1.511549	3.320749
1	1.940366	–2.287993	2.296496
1	1.841699	–0.557749	2.597981
6	4.345752	0.061732	1.680286
1	4.899576	–0.247123	2.575348
1	3.765607	0.945607	1.946340
1	5.089937	0.350577	0.938282
6	2.548366	2.607418	–2.001848
1	2.092940	1.908957	–2.707933
1	3.231137	3.259214	–2.555116
1	1.759648	3.231434	–1.586027
6	3.958703	2.787883	0.099650
1	4.078504	3.780702	–0.344279
1	4.951398	2.447635	0.394634
1	3.376550	2.894081	1.006211
6	4.488619	1.168299	–1.671814
1	4.181634	0.686098	–2.595920
1	5.027949	0.433650	–1.075644
1	5.191335	1.967905	–1.927016
6	–4.693906	1.821846	–0.450264
1	–4.350967	2.436318	0.383999
1	–5.779219	1.907667	–0.543808
1	–4.221500	2.198545	–1.359054
6	–4.939058	–0.810638	–1.559624
1	–4.468892	–0.501201	–2.494534
1	–6.014406	–0.625053	–1.616814
1	–4.762702	–1.879783	–1.429898
6	1.128747	3.841882	0.990749
1	1.722820	4.222367	0.161038
1	1.797341	3.682546	1.839220
1	0.439804	4.643857	1.283748
6	0.181052	–0.153250	0.139900
7	0.974291	–1.172385	0.017062
6	0.430216	–2.587004	–0.115407

6	1.498038	–3.681977	–0.005271
1	1.009781	–4.637174	–0.215111
1	2.303643	–3.560636	–0.720868
1	1.915263	–3.754545	0.997398
6	–0.224169	–2.720774	–1.497284
1	–1.004320	–1.970639	–1.649350
1	0.522370	–2.603799	–2.283605
1	–0.684683	–3.708275	–1.592893
6	–0.582775	–2.886232	1.004435
1	–0.763513	–3.963092	1.043033
1	–0.196947	–2.571598	1.975988
1	–1.550565	–2.405156	0.855174

CNtBu

SCF energy = –250.638223290

6	0.000000	0.000000	2.351017
7	0.000000	0.000000	1.182870
6	0.000000	0.000000	–0.258238
6	0.000000	1.456245	–0.731457
1	0.000000	1.492181	–1.823722
1	–0.885526	1.980622	–0.366560
1	0.885526	1.980622	–0.366560
6	–1.261145	–0.728123	–0.731457
1	–1.272506	–1.757199	–0.366560
1	–2.158032	–0.223423	–0.366560
1	–1.292267	–0.746091	–1.823722
6	1.261145	–0.728123	–0.731457
1	1.292267	–0.746091	–1.823722
1	2.158032	–0.223423	–0.366560
1	1.272506	–1.757199	–0.366560

4–3B1OI1

SCF energy = –2683.00426610

7	–2.817045	–0.963958	–1.294348
15	2.150184	1.042032	–0.163378
6	–2.177928	–1.362751	–2.562788
1	–2.988050	–1.713272	–3.207696
6	–1.197924	–2.539259	–2.461083
1	–0.291766	–2.249194	–1.922153
1	–0.903306	–2.865237	–3.464081
1	–1.648396	–3.389616	–1.948282
6	–4.203467	–1.452194	–1.168765
1	–4.516846	–1.201320	–0.157261
6	–5.164987	–0.747730	–2.127404
1	–6.196089	–1.055806	–1.931134
1	–4.947904	–0.974415	–3.176560
1	–5.113676	0.334755	–1.997940
79	–0.019344	0.013221	–0.134071
5	–2.091047	–0.579103	–0.079749
7	–2.937809	0.147324	0.981833
6	–2.920872	–0.194382	2.442833
6	–3.784443	–1.429702	2.735479
1	–4.828639	–1.223826	2.490376
1	–3.730180	–1.695421	3.796575
1	–3.460536	–2.291928	2.152758
6	–3.444336	0.965789	3.315779
1	–4.507367	1.156979	3.192994
1	–3.284400	0.718815	4.368480
1	–2.895698	1.889467	3.112900
6	–1.477509	–0.401198	2.940480
1	–1.491763	–0.570521	4.021360
1	–0.970806	–1.249328	2.488351
1	–0.879948	0.494177	2.745633
5	–3.771646	1.212069	0.540689
17	–5.585562	1.126699	0.900337
6	–3.303072	2.584580	–0.169936
6	–4.397161	3.659561	–0.241518
1	–4.806715	3.899827	0.743091
1	–5.232226	3.348080	–0.873748
1	–3.982265	4.581827	–0.666146
6	–2.135699	3.147424	0.668190
1	–2.461387	3.456673	1.666084
1	–1.709390	4.031480	0.178243
1	–1.340422	2.407079	0.784065
6	–2.782504	2.354774	–1.593470
1	–2.430153	3.303323	–2.020080
1	–3.559014	1.959756	–2.252645
1	–1.955766	1.649914	–1.604771
6	–4.334313	–2.976339	–1.284034
1	–5.356945	–3.277920	–1.038904
1	–4.121505	–3.344021	–2.292940
1	–3.662783	–3.481832	–0.586158
6	–1.523587	–0.219729	–3.340619
1	–1.129156	–0.600517	–4.288585
1	–2.241720	0.568517	–3.566523
1	–0.688402	0.218996	–2.786768
6	3.526640	–0.079503	–0.681242
6	3.231987	–0.700718	–2.057532
6	4.316094	–1.693229	–2.482037
6	4.532534	–2.775939	–1.426620
6	4.845340	–2.149847	–0.069875
6	3.737381	–1.189130	0.361882

1	4.451422	0.507660	–0.754038
1	3.137480	0.076260	–2.821182
1	2.261496	–1.211769	–2.015625
1	4.045077	–2.143017	–3.441966
1	5.259138	–1.155426	–2.644128
1	5.334309	–3.454773	–1.732500
1	3.621471	–3.383639	–1.342448
1	4.990047	–2.922122	0.691482
1	5.794366	–1.601704	–0.133116
1	3.978786	–0.768492	1.341255
1	2.795605	–1.740146	0.486510
6	1.681756	2.715515	2.045999
6	2.639838	1.637343	1.519138
6	4.097854	2.053752	1.757926
1	2.450460	0.737273	2.121866
6	1.919207	2.966130	3.535313
1	0.641731	2.426399	1.871954
1	1.845587	3.650199	1.496760
6	3.375098	3.342961	3.811982
1	1.247184	3.752950	3.890775
1	1.660612	2.058369	4.095407
6	4.341444	2.299033	3.250151
1	3.538055	3.471093	4.886395
1	3.587866	4.314518	3.346870
1	5.377320	2.613745	3.411079
1	4.214361	1.353838	3.794141
1	4.795001	1.295467	1.390539
1	4.320825	2.971306	1.205800
6	2.192171	2.425936	–1.390174
1	2.172857	1.881157	–2.344244
6	0.910206	3.274040	–1.361210
1	0.848366	3.831669	–0.420873
1	0.030898	2.628442	–1.389455
6	0.877938	4.254068	–2.533504
1	0.805535	3.689076	–3.471876
1	–0.025523	4.868736	–2.473046
6	2.125559	5.137211	–2.565451
1	2.103221	5.798629	–3.437074
1	2.129866	5.787911	–1.680966
6	3.402236	4.295115	–2.572647
1	3.458567	3.725564	–3.509425
1	4.285241	4.941659	–2.547209
6	3.433415	3.324748	–1.388979
1	3.453530	3.907260	–0.460887
1	4.353788	2.732247	–1.410280
6	–1.585568	–2.420839	0.677081
7	–0.796250	–3.288391	0.655502
6	0.469992	–3.912125	0.439842
1	1.032051	–3.238287	–0.224077
6	0.302373	–5.268461	–0.245517
1	–0.351990	–5.892913	0.373753
1	–0.197993	–5.130469	–1.207187
6	1.657431	–5.951896	–0.428138
1	2.271254	–5.364956	–1.123447
1	1.515406	–6.931316	–0.893301
6	2.394948	–6.091345	0.904094
1	3.373165	–6.556356	0.749514
1	1.828449	–6.761727	1.562684
6	2.558289	–4.731147	1.582764
1	3.207976	–4.101977	0.965299
1	3.057270	–4.839577	2.550042
6	1.213801	–4.031225	1.771915
1	1.345641	–3.032681	2.199854
1	0.587678	–4.599775	2.468916

4–3B1OTS

SCF energy = –2683.00426610

7	–2.817045	–0.963958	–1.294348
15	2.150184	1.042032	–0.163378
6	–2.177928	–1.362751	–2.562788
1	–2.988050	–1.713272	–3.207696
6	–1.197924	–2.539259	–2.461083
1	–0.291766	–2.249194	–1.922153
1	–0.903306	–2.865237	–3.464081
1	–1.648396	–3.389616	–1.948282
6	–4.203467	–1.452194	–1.168765
1	–4.516846	–1.201320	–0.157261
6	–5.164987	–0.747730	–2.127404
1	–6.196089	–1.055806	–1.931134
1	–4.947904	–0.974415	–3.176560
1	–5.113676	0.334755	–1.997940
79	–0.019344	0.013221	–0.134071
5	–2.091047	–0.579103	–0.079749
7	–2.937809	0.147324	0.981833
6	–2.920872	–0.194382	2.442833
6	–3.784443	–1.429702	2.735479
1	–4.828639	–1.223826	2.490376
1	–3.730180	–1.695421	3.796575
1	–3.460536	–2.291928	2.152758
6	–3.444336	0.965789	3.315779
1	–4.507367	1.156979	3.192994
1	–3.284400	0.718815	4.368480
1	–2.895698	1.889467	3.112900

6	–1.477509	–0.401198	2.940480	1	2.450460	0.737273	2.121866
1	–1.491763	–0.570521	4.021360	6	1.919207	2.966130	3.535313
1	–0.970806	–1.249328	2.488351	1	0.641731	2.426399	1.871954
1	–0.879948	0.494177	2.745633	1	1.845587	3.650199	1.496760
5	–3.771646	1.212069	0.540689	6	3.375098	3.342961	3.811982
17	–5.585562	1.126699	0.900337	1	1.247184	3.752950	3.890775
6	–3.303072	2.584580	–0.169936	1	1.660612	2.058369	4.095407
6	–4.397161	3.659561	–0.241518	6	4.341444	2.299033	3.250151
1	–4.806715	3.899827	0.743091	1	3.538055	3.471093	4.886395
1	–5.232226	3.348080	–0.873748	1	3.587866	4.314518	3.346870
1	–3.982265	4.581827	–0.666146	1	5.377320	2.613745	3.411079
6	–2.135699	3.147424	0.668190	1	4.214361	1.353838	3.794141
1	–2.461387	3.456673	1.666084	1	4.795001	1.295467	1.390539
1	–1.709390	4.031480	0.178243	1	4.320825	2.971306	1.205800
1	–1.340422	2.407079	0.784065	6	2.192171	2.425936	–1.390174
6	–2.782504	2.354774	–1.593470	1	2.172857	1.881157	–2.344244
1	–2.430153	3.303323	–2.020080	6	0.910206	3.274040	–1.361210
1	–3.559014	1.959756	–2.252645	1	0.848366	3.831669	–0.420873
1	–1.955766	1.649914	–1.604771	1	0.030898	2.628442	–1.389455
6	–4.334313	–2.976339	–1.284034	6	0.877938	4.254068	–2.533504
1	–5.356945	–3.277920	–1.038904	1	0.805535	3.689076	–3.471876
1	–4.121505	–3.344021	–2.292940	1	–0.025523	4.868736	–2.473046
1	–3.662783	–3.481832	–0.586158	6	2.125559	5.137211	–2.565451
6	–1.523587	–0.219729	–3.340619	1	2.103221	5.798629	–3.437074
1	–1.129156	–0.600517	–4.288585	1	2.129866	5.787911	–1.680966
1	–2.241720	0.568517	–3.566523	6	3.402236	4.295115	–2.572647
1	–0.688402	0.218996	–2.786768	1	3.458567	3.725564	–3.509425
6	3.526640	–0.079503	–0.681242	1	4.285241	4.941659	–2.547209
6	3.231987	–0.700718	–2.057532	6	3.433415	3.324748	–1.388979
6	4.316094	–1.693229	–2.482037	1	3.453530	3.907260	–0.460887
6	4.532534	–2.775939	–1.426620	1	4.353788	2.732247	–1.410280
6	4.845340	–2.149847	–0.069875	6	–1.585568	–2.420839	0.677081
6	3.737381	–1.189130	0.361882	7	–0.796250	–3.288391	0.655502
1	4.451422	0.507660	–0.754038	6	0.469992	–3.912125	0.439842
1	3.137480	0.076260	–2.821182	1	1.032051	–3.238287	–0.224077
1	2.261496	–1.211769	–2.015625	6	0.302373	–5.268461	–0.245517
1	4.045077	–2.143017	–3.441966	1	–0.351990	–5.892913	0.373753
1	5.259138	–1.155426	–2.644128	1	–0.197993	–5.130469	–1.207187
1	5.334309	–3.454773	–1.732500	6	1.657431	–5.951896	–0.428138
1	3.621471	–3.383639	–1.342448	1	2.271254	–5.364956	–1.123447
1	4.990047	–2.922122	0.691482	1	1.515406	–6.931316	–0.893301
1	5.794366	–1.601704	–0.133116	6	2.394948	–6.091345	0.904094
1	3.978786	–0.768492	1.341255	1	3.373165	–6.556356	0.749514
1	2.795605	–1.740146	0.486510	1	1.828449	–6.761727	1.562684
6	1.681756	2.715515	2.045999	6	2.558289	–4.731147	1.582764
6	2.639838	1.637343	1.519138	1	3.207976	–4.101977	0.965299
6	4.097854	2.053752	1.757926	1	3.057270	–4.839577	2.550042

6	1.213801	–4.031225	1.771915
1	1.345641	–3.032681	2.199854
1	0.587678	–4.599775	2.468916

4–3B1OiI1

SCF energy = –2683.05284605

7	–4.058838	0.736731	–1.138235
15	2.431250	–0.193637	–0.506892
6	–4.005065	2.095740	–1.720646
1	–4.788986	2.113802	–2.482645
6	–2.695938	2.347972	–2.471273
1	–1.848177	2.455788	–1.793427
1	–2.777003	3.270847	–3.053475
1	–2.477156	1.528800	–3.162736
6	–5.363233	0.060428	–1.259914
1	–5.191925	–0.950201	–0.889189
6	–6.433125	0.680113	–0.355289
1	–7.302651	0.017068	–0.308319
1	–6.779904	1.642891	–0.740692
1	–6.053118	0.822950	0.655721
79	0.166549	0.362537	–0.200776
5	–2.998557	0.145926	–0.419650
7	–2.905617	–1.354469	–0.134581
6	–2.571348	–2.337626	–1.217082
6	–3.252743	–1.972168	–2.541783
1	–4.334655	–2.074005	–2.483733
1	–2.901785	–2.659326	–3.316439
1	–3.012350	–0.957870	–2.860754
6	–3.126020	–3.713919	–0.828051
1	–4.195371	–3.636278	–0.613820
1	–2.995887	–4.421443	–1.651795
1	–2.640100	–4.140408	0.045755
6	–1.071767	–2.419103	–1.539527
1	–0.877972	–3.266584	–2.205379
1	–0.740238	–1.511396	–2.051524
1	–0.462786	–2.537515	–0.651834
5	–2.918618	–1.644564	1.250615
17	–4.150771	–0.628244	2.160474
6	–2.076515	–2.595646	2.255241
6	–2.968234	–3.703666	2.845400
1	–3.295736	–4.422979	2.089204
1	–3.862122	–3.287936	3.316297
1	–2.417859	–4.262392	3.612031
6	–0.785466	–3.218674	1.703139
1	–0.931834	–3.924825	0.886128
1	–0.275583	–3.766411	2.504360
1	–0.099559	–2.437113	1.365070
6	–1.590199	–1.699267	3.423424
1	–0.945634	–2.287565	4.086994
1	–2.409572	–1.299908	4.019692
1	–1.003379	–0.853697	3.053584
6	–5.903381	–0.025070	–2.696055
1	–6.627377	–0.842147	–2.767504
1	–6.430520	0.886630	–2.990032
1	–5.117571	–0.206856	–3.429958
6	–4.307060	3.236541	–0.744486
1	–4.321972	4.188428	–1.286769
1	–5.276892	3.109387	–0.263145
1	–3.554765	3.272426	0.040973
6	3.287045	1.082610	–1.534892
6	3.324741	2.454076	–0.842519
6	3.943024	3.524295	–1.743685
6	3.229848	3.611929	–3.091249
6	3.220695	2.252882	–3.788688
6	2.585114	1.183763	–2.900612
1	4.321972	0.756194	–1.694343
1	3.893030	2.399632	0.090454
1	2.305829	2.753781	–0.571503
1	3.913034	4.490826	–1.231566
1	5.003214	3.291748	–1.909490
1	3.707926	4.363958	–3.726176
1	2.195723	3.943655	–2.933402
1	2.679034	2.311973	–4.737544
1	4.250939	1.961901	–4.033282
1	2.598422	0.217263	–3.414519
1	1.528380	1.429982	–2.737202
6	2.456174	–3.005651	–0.485194
6	2.749420	–1.794867	–1.381824
6	4.108414	–1.973788	–2.073325
1	1.975968	–1.781527	–2.162510
6	2.446865	–4.296651	–1.301765
1	1.508012	–2.882005	0.039732
1	3.233606	–3.081702	0.283833
6	3.779396	–4.492621	–2.024583
1	2.236944	–5.148044	–0.647263
1	1.629703	–4.253774	–2.032782
6	4.129748	–3.275786	–2.881445
1	3.750891	–5.394622	–2.643459
1	4.570667	–4.650357	–1.279948
1	5.112249	–3.406739	–3.345437
1	3.406054	–3.192754	–3.702714
1	4.326249	–1.137654	–2.742429
1	4.907719	–1.992314	–1.324232

6	3.287876	–0.141933	1.126723
1	3.159463	0.917260	1.388462
6	2.565073	–0.925600	2.234973
1	2.648573	–2.002392	2.059929
1	1.497036	–0.694132	2.233115
6	3.173500	–0.591962	3.597127
1	2.996746	0.469005	3.816814
1	2.664133	–1.161281	4.380279
6	4.676029	–0.875841	3.619612
1	5.102492	–0.599838	4.588673
1	4.839511	–1.955220	3.502851
6	5.401225	–0.134819	2.495135
1	5.337344	0.946426	2.673900
1	6.465928	–0.388414	2.494582
6	4.788799	–0.447693	1.127119
1	4.944058	–1.508757	0.897463
1	5.305587	0.121368	0.347603
6	–1.777694	0.978387	0.192855
7	–2.127232	1.886166	1.030507
6	–1.164289	2.709823	1.771891
1	–1.780396	3.407401	2.355920
6	–0.281783	3.568131	0.854837
1	0.265048	2.911591	0.169666
1	–0.924291	4.198640	0.230849
6	0.714398	4.419080	1.641163
1	0.172759	5.176738	2.222481
1	1.365424	4.967448	0.951034
6	1.547662	3.564979	2.597441
1	2.250610	4.192034	3.155851
1	2.152004	2.855950	2.014057
6	0.645153	2.786491	3.554508
1	0.096083	3.496334	4.186880
1	1.244603	2.168910	4.232319
6	–0.341667	1.909989	2.787764
1	–1.026998	1.400493	3.471377
1	0.215769	1.128017	2.260270

4–3B1iTS

SCF energy = –2683.01119282

7	–2.910575	0.256729	–1.801000
15	2.382531	–0.247109	–0.231996
6	–2.344897	1.177938	–2.794521
1	–3.188846	1.579013	–3.361231
6	–1.457997	0.454668	–3.809600
1	–0.587801	0.010862	–3.318135
1	–1.102715	1.145826	–4.581803
1	–2.013879	–0.349628	–4.298413
6	–4.377964	0.236144	–1.752949
1	–4.632529	–0.554114	–1.048576
6	–4.950436	1.544590	–1.198886
1	–6.034285	1.467972	–1.070557
1	–4.753552	2.386423	–1.872663
1	–4.515378	1.771587	–0.223899
79	0.018723	–0.265362	–0.599576
5	–2.130914	–0.402067	–0.772757
7	–2.687063	–1.632250	–0.046697
6	–2.560192	–2.968270	–0.682290
6	–3.290289	–2.951668	–2.033421
1	–4.349192	–2.721757	–1.895990
1	–3.211628	–3.929583	–2.519324
1	–2.860033	–2.202383	–2.698395
6	–3.250135	–4.029937	0.182124
1	–4.269988	–3.725091	0.435440
1	–3.310814	–4.975618	–0.363203
1	–2.709271	–4.228169	1.106854
6	–1.111397	–3.412393	–0.952323
1	–1.104205	–4.433063	–1.348949
1	–0.630092	–2.766225	–1.690281
1	–0.506286	–3.396022	–0.046339
5	–3.068817	–1.438968	1.311202
17	–4.729471	–0.643012	1.645169
6	–2.350054	–1.885265	2.695635
6	–3.231116	–2.833234	3.532401
1	–3.482764	–3.754932	3.002739
1	–4.168747	–2.353450	3.820072
1	–2.703592	–3.117472	4.451271
6	–0.975870	–2.530675	2.467225
1	–1.042556	–3.525137	2.022838
1	–0.444931	–2.641588	3.420944
1	–0.358895	–1.912287	1.809533
6	–2.093996	–0.633265	3.568961
1	–1.722319	–0.948528	4.551632
1	–2.998884	–0.043219	3.725547
1	–1.334303	0.017979	3.130178
6	–5.042216	–0.112645	–3.089862
1	–6.103293	–0.324645	–2.927920
1	–4.989997	0.705479	–3.815250
1	–4.589196	–0.994654	–3.545027
6	–1.633981	2.397198	–2.201905
1	–1.374726	3.111717	–2.990583
1	–2.276415	2.903085	–1.477389
1	–0.714118	2.100479	–1.693580
6	3.274351	0.786284	–1.479371

6	2.772005	2.239503	–1.434487
6	3.402840	3.100105	–2.529565
6	3.172033	2.497517	–3.913820
6	3.692132	1.062981	–3.971623
6	3.056874	0.196428	–2.883980
1	4.348544	0.777052	–1.251878
1	2.972487	2.692156	–0.458816
1	1.682489	2.238434	–1.560780
1	2.989635	4.112514	–2.479143
1	4.481499	3.192667	–2.347345
1	3.653479	3.110357	–4.681979
1	2.096769	2.500707	–4.134043
1	3.493276	0.621850	–4.952977
1	4.782883	1.065815	–3.844535
1	3.458875	–0.818867	–2.944736
1	1.978476	0.114828	–3.069860
6	2.581878	–2.884568	0.693492
6	3.086340	–1.946817	–0.413570
6	4.601395	–2.100425	–0.602006
1	2.603782	–2.279340	–1.343581
6	2.923059	–4.337967	0.365422
1	1.503598	–2.770936	0.830241
1	3.052053	–2.614146	1.646703
6	4.423757	–4.517862	0.132211
1	2.581967	–4.991682	1.173892
1	2.370166	–4.638928	–0.533382
6	4.945441	–3.555329	–0.936037
1	4.642926	–5.552055	–0.150441
1	4.957549	–4.333122	1.073882
1	6.028240	–3.665893	–1.051206
1	4.500534	–3.813406	–1.905793
1	4.969387	–1.443184	–1.394989
1	5.126616	–1.808542	0.312209
6	2.851250	0.474103	1.406715
1	2.715496	1.548726	1.228389
6	1.854725	0.092532	2.513873
1	1.929370	–0.977219	2.736392
1	0.829186	0.254783	2.171226
6	2.120507	0.898398	3.784505
1	1.920105	1.960383	3.583804
1	1.421585	0.592040	4.568648
6	3.565196	0.738272	4.259024
1	3.747392	1.354993	5.144377
1	3.728294	–0.303066	4.565599
6	4.558189	1.094920	3.151459
1	4.473571	2.164537	2.918185
1	5.584764	0.930438	3.493360
6	4.295030	0.281190	1.881485
1	4.470017	–0.778279	2.099056
1	5.005406	0.564364	1.098201
6	–2.131160	0.898427	0.804537
7	–1.845632	1.929983	1.274403
6	–1.204534	3.121478	1.720560
1	–1.076532	3.014956	2.805170
6	–2.077107	4.347686	1.443355
1	–2.268816	4.401803	0.366042
1	–3.044902	4.229514	1.937132
6	–1.368686	5.618924	1.913911
1	–1.268155	5.595094	3.006651
1	–1.985795	6.490602	1.679179
6	0.017576	5.762105	1.281665
1	0.514749	6.658554	1.663599
1	–0.092235	5.899842	0.198658
6	0.876717	4.523896	1.545322
1	1.085397	4.444352	2.620377
1	1.846568	4.617375	1.046635
6	0.173581	3.256734	1.066531
1	0.762068	2.364675	1.285225
1	0.040818	3.287589	–0.018692

4–3B2ClO1

SCF energy = –2683.03065916

7	–0.255505	3.639524	0.213388
15	2.627103	–1.113182	0.022216
6	0.973783	4.270493	0.730271
1	0.744881	5.331304	0.857766
6	2.135478	4.205844	–0.262786
1	2.482028	3.177896	–0.396299
1	2.977020	4.810149	0.092471
1	1.826973	4.587193	–1.239415
6	–1.351041	4.590403	–0.046686
1	–2.151705	3.998209	–0.485222
6	–1.900459	5.215989	1.234362
1	–2.769558	5.839102	1.005402
1	–1.160038	5.848349	1.736585
1	–2.225631	4.443759	1.929939
79	1.177016	0.808871	0.118574
5	–0.375307	2.249888	–0.041719
7	–1.686373	1.708647	–0.561663
6	–1.715624	1.453071	–2.028695
6	–3.056222	1.868890	–2.658090
1	–3.913844	1.295918	–2.304770
1	–3.010387	1.740229	–3.744377

1	–3.265643	2.917827	–2.440828	1	3.571935	–0.841477	–2.767084
6	–1.403713	–0.025542	–2.344199	1	3.523463	0.742038	–2.015528
1	–2.111094	–0.716036	–1.880225	6	0.509746	–2.857100	–0.619463
1	–1.417619	–0.212911	–3.423633	6	1.839607	–2.309620	–1.158323
1	–0.409652	–0.275778	–1.964179	6	2.693061	–3.441374	–1.745947
6	–0.647263	2.288468	–2.757467	1	1.579054	–1.637839	–1.988404
1	–0.691669	2.084044	–3.831269	6	–0.261181	–3.587296	–1.719034
1	–0.819524	3.354274	–2.611625	1	–0.098607	–2.047021	–0.210225
1	0.363545	2.058245	–2.414084	1	0.706025	–3.555959	0.202305
5	–2.776327	1.289307	0.327743	6	0.578576	–4.700734	–2.346051
17	–4.280791	2.666327	0.487278	1	–1.189545	–3.999321	–1.308424
6	–2.503993	0.672961	1.852899	1	–0.551745	–2.863167	–2.490380
6	–1.708516	1.642974	2.735554	6	1.920695	–4.168836	–2.850907
1	–2.231654	2.594578	2.850037	1	0.030387	–5.179126	–3.163843
1	–0.714957	1.847123	2.337233	1	0.761132	–5.480201	–1.594436
1	–1.576842	1.213920	3.737720	1	2.527059	–4.987243	–3.251633
6	–3.798693	0.345319	2.620433	1	1.746214	–3.472812	–3.681718
1	–4.398182	1.238630	2.799736	1	3.631316	–3.054817	–2.153273
1	–3.551863	–0.100199	3.591916	1	2.964140	–4.158332	–0.964949
1	–4.435589	–0.376672	2.096329	6	2.953319	–1.924600	1.650881
6	–1.700650	–0.633135	1.730418	1	3.671399	–1.231784	2.110361
1	–1.478562	–1.046961	2.722222	6	1.714738	–1.914104	2.563000
1	–0.749005	–0.465903	1.222591	1	0.928218	–2.549605	2.142355
1	–2.241813	–1.410249	1.175492	1	1.295143	–0.905848	2.614581
6	–0.972059	5.682152	–1.053873	6	2.067921	–2.408604	3.966808
1	–1.867724	6.239707	–1.342696	1	2.750365	–1.689701	4.438559
1	–0.260199	6.406374	–0.645189	1	1.166114	–2.432603	4.586384
1	–0.531320	5.262192	–1.960315	6	2.730805	–3.786024	3.934163
6	1.375515	3.770031	2.116994	1	3.007633	–4.098396	4.945927
1	2.209796	4.363591	2.505409	1	2.008472	–4.526589	3.565781
1	0.538837	3.857283	2.814460	6	3.958753	–3.788068	3.023368
1	1.686139	2.722703	2.089068	1	4.725844	–3.124788	3.443680
6	4.294083	–0.792368	–0.708477	1	4.401291	–4.788257	2.978563
6	5.124906	0.138030	0.188901	6	3.600111	–3.313039	1.613254
6	6.471136	0.483278	–0.451111	1	2.895792	–4.028098	1.172896
6	6.295411	1.095151	–1.839474	1	4.490202	–3.312824	0.975570
6	5.475421	0.172888	–2.739538	6	–3.733574	0.140111	–0.296649
6	4.127203	–0.169931	–2.105892	7	–4.429592	–0.734154	–0.573689
1	4.827766	–1.746567	–0.805926	6	–5.256636	–1.870405	–0.825379
1	5.300845	–0.322695	1.165071	1	–5.386176	–1.925312	–1.911757
1	4.557207	1.059322	0.372763	6	–6.620936	–1.681954	–0.156123
1	7.023217	1.166779	0.201260	1	–6.463023	–1.521227	0.915822
1	7.076689	–0.429238	–0.531207	1	–7.100780	–0.781929	–0.547509
1	7.270767	1.299950	–2.291566	6	–7.490220	–2.919294	–0.383163
1	5.781884	2.060578	–1.747249	1	–7.717042	–3.015233	–1.452596
1	5.314211	0.637465	–3.717155	1	–8.448600	–2.786565	0.125248
1	6.036920	–0.753236	–2.921260	6	–6.794675	–4.191157	0.105102

1	–7.420013	–5.065075	–0.097739
1	–6.669356	–4.139818	1.193718
6	–5.424195	–4.361083	–0.552695
1	–5.553575	–4.527861	–1.629521
1	–4.918132	–5.247129	–0.160358
6	–4.542145	–3.132565	–0.330180
1	–3.581563	–3.236175	–0.842639
1	–4.327434	–3.010192	0.737362

4–3B2ClOTS

SCF energy = –2683.01694392

7	0.455897	–3.616099	–0.340561
15	–2.582883	0.998192	–0.009850
6	–0.835404	–4.333133	–0.313064
1	–0.599078	–5.395119	–0.411135
6	–1.733317	–3.987663	–1.502724
1	–2.085720	–2.954913	–1.441620
1	–2.606337	–4.648683	–1.526271
1	–1.191301	–4.103490	–2.444332
6	1.616925	–4.492620	–0.588927
1	2.469486	–3.825093	–0.699622
6	1.918854	–5.417456	0.589008
1	2.794991	–6.034474	0.369554
1	1.084199	–6.092220	0.807969
1	2.139338	–4.840136	1.485946
79	–1.036759	–0.839405	–0.057191
5	0.569547	–2.208226	–0.194165
7	1.967985	–1.612724	–0.211817
6	2.369808	–1.014312	–1.517762
6	3.871132	–1.144365	–1.810612
1	4.504279	–0.629538	–1.091083
1	4.078407	–0.720048	–2.798701
1	4.174816	–2.192214	–1.817695
6	1.949935	0.472395	–1.560382
1	2.293379	1.013330	–0.679775
1	2.349405	0.968970	–2.452575
1	0.859829	0.556072	–1.585769
6	1.654193	–1.709070	–2.688940
1	1.897798	–1.191869	–3.621878
1	1.977364	–2.745017	–2.789009
1	0.567897	–1.695363	–2.575563
5	2.727303	–1.586323	1.011250
17	4.327676	–2.595507	1.038381
6	2.103482	–1.338566	2.497380
6	1.152492	–2.478078	2.909061
1	1.649719	–3.450439	2.887178
1	0.271981	–2.534523	2.269208
1	0.801879	–2.313921	3.935935
6	3.184868	–1.251705	3.587157
1	3.707451	–2.201003	3.719289
1	2.723690	–0.985973	4.546488
1	3.939280	–0.492597	3.359943
6	1.298053	–0.027184	2.540194
1	0.767342	0.063748	3.496449
1	0.551784	0.015920	1.743867
1	1.942322	0.851832	2.443313
6	1.491502	–5.302033	–1.885569
1	2.457752	–5.753389	–2.128009
1	0.767840	–6.118919	–1.806433
1	1.191369	–4.674573	–2.726962
6	–1.574305	–4.202665	1.017875
1	–2.457878	–4.849578	1.021985
1	–0.928182	–4.501330	1.846666
1	–1.903290	–3.175886	1.195497
6	–4.041953	0.769460	–1.122331
6	–4.881375	–0.436591	–0.668483
6	–6.028210	–0.734508	–1.636612
6	–5.520116	–0.939747	–3.062032
6	–4.710611	0.269343	–3.524609
6	–3.554892	0.564199	–2.568096
1	–4.669428	1.669484	–1.082610
1	–5.292458	–0.267475	0.330906
1	–4.229142	–1.316124	–0.594661
1	–6.573419	–1.619097	–1.293379
1	–6.743225	0.098573	–1.622146
1	–6.356619	–1.122995	–3.743388
1	–4.884882	–1.834134	–3.094705
1	–4.317113	0.105063	–4.532476
1	–5.368252	1.146809	–3.583548
1	–3.005086	1.441381	–2.920869
1	–2.845718	–0.273322	–2.586803
6	–0.532656	2.907755	0.208192
6	–1.694892	2.472940	–0.697881
6	–2.518605	3.687236	–1.147919
1	–1.236123	2.039817	–1.598134
6	0.357488	3.927197	–0.502134
1	0.059476	2.040535	0.514439
1	–0.931320	3.360211	1.124093
6	–0.446591	5.131681	–0.991470
1	1.154029	4.254389	0.173054
1	0.847479	3.438287	–1.354566
6	–1.622942	4.699976	–1.867853
1	0.199787	5.823848	–1.540489

1	–0.829794	5.684097	–0.123398
1	–2.212973	5.571587	–2.168455
1	–1.240306	4.247705	–2.792182
1	–3.335275	3.384482	–1.809232
1	–2.982818	4.171203	–0.283872
6	–3.283983	1.375864	1.659682
1	–4.038384	0.586580	1.779997
6	–2.248883	1.152113	2.776214
1	–1.428688	1.871790	2.680893
1	–1.795908	0.162704	2.673463
6	–2.890637	1.297094	4.156611
1	–3.615133	0.485460	4.303334
1	–2.127038	1.175481	4.930913
6	–3.602386	2.640866	4.313461
1	–4.081814	2.706536	5.294992
1	–2.861049	3.449859	4.273218
6	–4.633786	2.850199	3.204377
1	–5.429978	2.100635	3.300975
1	–5.112125	3.829506	3.306113
6	–3.988143	2.727254	1.822401
1	–3.252521	3.531586	1.711388
1	–4.738512	2.874254	1.038634
6	3.875014	0.397894	0.991267
7	4.482787	1.364459	0.774093
6	5.100437	2.553381	0.276114
1	5.834448	2.876389	1.021876
6	4.034246	3.638719	0.097890
1	3.260111	3.247643	–0.570717
1	3.555248	3.843159	1.059429
6	4.642905	4.907004	–0.498253
1	5.351790	5.344463	0.216298
1	3.856013	5.651609	–0.649731
6	5.363474	4.611305	–1.814455
1	5.823807	5.522462	–2.207242
1	4.630276	4.282291	–2.561607
6	6.420337	3.520777	–1.631805
1	7.212449	3.888091	–0.966869
1	6.900599	3.289502	–2.586364
6	5.813095	2.246355	–1.045060
1	6.577076	1.481805	–0.882514
1	5.079143	1.823459	–1.740441

4–3B2CliI1

SCF energy = –2683.03871782

7	2.604442	–1.087479	1.825372
15	–2.511612	–0.280845	–0.022942
6	1.960639	–0.851027	3.129627
1	2.744209	–0.949717	3.884259
6	0.910028	–1.905568	3.476985
1	0.050977	–1.839720	2.806562
1	0.559691	–1.774318	4.506522
1	1.333098	–2.908294	3.381477
6	4.053097	–1.348719	1.920003
1	4.372296	–1.565349	0.902429
6	4.832792	–0.120658	2.392407
1	5.907376	–0.314353	2.341251
1	4.591779	0.147758	3.427710
1	4.630393	0.740219	1.753261
79	–0.157015	–0.702705	0.323279
5	1.914809	–1.098482	0.578265
7	2.703387	–1.304843	–0.682332
6	2.605508	–2.651254	–1.289186
6	3.922221	–3.036261	–1.974573
1	4.210908	–2.340890	–2.758926
1	3.836861	–4.032907	–2.420634
1	4.735188	–3.050527	–1.245252
6	1.423404	–2.793801	–2.268516
1	1.516338	–2.141379	–3.133717
1	1.347023	–3.822528	–2.636373
1	0.485114	–2.547434	–1.761342
6	2.373413	–3.698632	–0.183743
1	2.321104	–4.698254	–0.625193
1	3.191177	–3.692564	0.536923
1	1.437410	–3.524617	0.355646
5	3.299357	–0.093050	–1.300873
17	5.285476	0.005212	–1.138312
6	2.911673	0.550119	–2.800744
6	3.539804	1.943522	–3.018408
1	4.629988	1.897055	–3.011553
1	3.237374	2.675930	–2.262648
1	3.224339	2.347585	–3.988315
6	3.403534	–0.295695	–3.985716
1	4.484115	–0.452070	–3.933443
1	3.192950	0.227258	–4.927348
1	2.924802	–1.271214	–4.054049
6	1.386702	0.725698	–2.894949
1	1.089488	1.063628	–3.895985
1	1.038143	1.486573	–2.187466
1	0.839232	–0.189924	–2.666031
6	4.389856	–2.565688	2.788231
1	5.440694	–2.833949	2.648309
1	4.246002	–2.378330	3.857197
1	3.782055	–3.431440	2.517828

6	1.422273	0.570840	3.284748
1	1.026647	0.726841	4.293801
1	2.224174	1.295152	3.117494
1	0.621744	0.763928	2.568219
6	–3.413878	–0.343149	1.592349
6	–2.901637	0.753802	2.541450
6	–3.551690	0.661911	3.922942
6	–3.356883	–0.720917	4.541231
6	–3.897311	–1.806940	3.613076
6	–3.244333	–1.731306	2.232971
1	–4.482547	–0.173565	1.410518
1	–3.087988	1.746306	2.119393
1	–1.813979	0.653416	2.647355
1	–3.136419	1.436009	4.576000
1	–4.625820	0.870958	3.833187
1	–3.846776	–0.774376	5.518264
1	–2.286634	–0.893254	4.713241
1	–3.728609	–2.798146	4.044733
1	–4.984338	–1.690223	3.510260
1	–3.662442	–2.507968	1.586120
1	–2.174631	–1.950956	2.329388
6	–2.752434	–1.613772	–2.485261
6	–3.279126	–1.619331	–1.042344
6	–4.805288	–1.772943	–1.028917
1	–2.854072	–2.513071	–0.563090
6	–3.148357	–2.900751	–3.208552
1	–1.665773	–1.483002	–2.501205
1	–3.183852	–0.762368	–3.024114
6	–4.664218	–3.102790	–3.183504
1	–2.783934	–2.874195	–4.239922
1	–2.653321	–3.752148	–2.724868
6	–5.213935	–3.058110	–1.756373
1	–4.929692	–4.051173	–3.660541
1	–5.141500	–2.311523	–3.776660
1	–6.304671	–3.150002	–1.766435
1	–4.834028	–3.921438	–1.194762
1	–5.193053	–1.791370	–0.006158
1	–5.272145	–0.914734	–1.523538
6	–2.900279	1.395828	–0.698684
1	–2.511192	2.040811	0.102383
6	–2.078671	1.741011	–1.948896
1	–2.418175	1.144463	–2.800770
1	–1.030754	1.479059	–1.794409
6	–2.224114	3.222439	–2.299696
1	–1.791751	3.833223	–1.496133
1	–1.651042	3.447253	–3.204570
6	–3.692027	3.609244	–2.485404
1	–3.781759	4.680435	–2.690745
1	–4.093078	3.088960	–3.364815
6	–4.526403	3.235665	–1.258869
1	–4.205502	3.842396	–0.401264
1	–5.581220	3.472247	–1.429771
6	–4.375334	1.753169	–0.906932
1	–4.780722	1.150031	–1.727099
1	–4.968787	1.516749	–0.018405
6	2.860736	1.148738	–0.319579
7	2.472320	2.088794	0.218574
6	1.793285	3.206159	0.795877
1	1.999366	3.174254	1.870171
6	0.288542	3.050613	0.556531
1	0.121520	2.990554	–0.523610
1	–0.057062	2.105621	0.980476
6	–0.468402	4.240064	1.140421
1	–0.360040	4.242000	2.232341
1	–1.537795	4.124436	0.937528
6	0.047925	5.560559	0.567971
1	–0.477088	6.404893	1.023899
1	–0.170480	5.597763	–0.507039
6	1.556589	5.702637	0.781645
1	1.765979	5.784873	1.855682
1	1.922291	6.625854	0.324665
6	2.325471	4.513301	0.203127
1	3.396654	4.603333	0.399975
1	2.198525	4.477524	–0.884661

4–3B2CliTS

SCF energy = –2683.02278098

7	2.753484	–0.538485	1.902943
15	–2.407348	–0.462035	0.070137
6	2.079593	–0.082098	3.132190
1	2.860619	0.037452	3.886519
6	1.111671	–1.123778	3.693205
1	0.284894	–1.297488	3.002164
1	0.700848	–0.794413	4.653745
1	1.623797	–2.076726	3.846369
6	4.209541	–0.707144	2.055085
1	4.548633	–1.136453	1.114899
6	4.926589	0.631032	2.234147
1	6.010031	0.481937	2.250132
1	4.646797	1.123067	3.172632
1	4.695770	1.303094	1.406620
79	–0.012770	–0.596071	0.382802
5	2.086838	–0.789432	0.669436

7	2.903685	–1.286051	–0.502190	1	–4.449543	1.863659	3.404846
6	2.807857	–2.745053	–0.789949	1	–3.543784	0.919141	5.510494
6	4.086415	–3.245310	–1.473946	1	–2.001356	0.592328	4.728588
1	4.262935	–2.767727	–2.438766	1	–3.355835	–1.480504	4.812615
1	4.016626	–4.323143	–1.649594	1	–4.684446	–0.676233	3.988742
1	4.959677	–3.052259	–0.847717	1	–3.365773	–2.055056	2.407991
6	1.587049	–3.108299	–1.656658	1	–1.897720	–1.202578	2.843170
1	1.635049	–2.649305	–2.643541	6	–2.672790	–2.524952	–1.802976
1	1.521911	–4.192331	–1.796785	6	–3.099595	–2.116018	–0.385456
1	0.665007	–2.773444	–1.173578	6	–4.599947	–2.366683	–0.182195
6	2.676374	–3.525142	0.527331	1	–2.557946	–2.775916	0.307244
1	2.620193	–4.597727	0.319068	6	–3.002117	–3.993663	–2.069602
1	3.540723	–3.350586	1.168498	1	–1.604169	–2.340270	–1.950605
1	1.775754	–3.245138	1.080134	1	–3.206703	–1.905566	–2.533369
5	3.521197	–0.364308	–1.431107	6	–4.486359	–4.279527	–1.836907
17	5.360374	–0.085714	–1.246967	1	–2.719819	–4.256909	–3.093501
6	2.976075	0.181850	–2.860381	1	–2.396032	–4.623545	–1.406428
6	3.576289	1.537691	–3.275881	6	–4.929466	–3.839977	–0.441082
1	4.657719	1.477410	–3.408769	1	–4.695712	–5.343519	–1.983401
1	3.379645	2.322067	–2.541825	1	–5.078256	–3.739219	–2.587557
1	3.138491	1.858312	–4.229366	1	–6.003083	–4.008954	–0.311735
6	3.385792	–0.813488	–3.970664	1	–4.423452	–4.457727	0.312166
1	4.468819	–0.962539	–3.998448	1	–4.912825	–2.092137	0.828723
1	3.084143	–0.413525	–4.945968	1	–5.183555	–1.743342	–0.866605
1	2.912676	–1.790874	–3.867657	6	–2.977868	0.829229	–1.124494
6	1.447269	0.315105	–2.866559	1	–2.745588	1.749771	–0.575135
1	1.084371	0.579551	–3.868092	6	–2.126759	0.876670	–2.402429
1	1.121145	1.100087	–2.179898	1	–2.302974	–0.018599	–3.007335
1	0.946183	–0.603261	–2.557110	1	–1.065743	0.867448	–2.148183
6	4.591980	–1.682973	3.173385	6	–2.466194	2.115824	–3.231881
1	5.654726	–1.929112	3.094271	1	–2.174477	3.015978	–2.673933
1	4.433936	–1.266579	4.173293	1	–1.875304	2.117806	–4.152869
1	4.024459	–2.613529	3.105762	6	–3.959360	2.187250	–3.554619
6	1.434554	1.297769	2.999509	1	–4.185572	3.103872	–4.108128
1	1.006721	1.613124	3.957152	1	–4.226323	1.351004	–4.213771
1	2.183248	2.033859	2.697319	6	–4.807723	2.113460	–2.284084
1	0.639443	1.290822	2.250764	1	–4.626259	3.007687	–1.672933
6	–3.249315	–0.009906	1.656848	1	–5.873037	2.119635	–2.535169
6	–2.764851	1.363668	2.151876	6	–4.471589	0.866424	–1.462363
6	–3.364688	1.731365	3.509303	1	–4.733739	–0.022691	–2.047062
6	–3.083336	0.653726	4.553998	1	–5.081644	0.838151	–0.553984
6	–3.590214	–0.705465	4.076692	6	2.705305	1.705459	–0.284842
6	–2.980488	–1.082330	2.726070	7	2.052716	2.626325	–0.002034
1	–4.331187	0.046164	1.478705	6	1.088964	3.633823	0.296957
1	–3.009318	2.146138	1.427841	1	1.054165	3.723759	1.388936
1	–1.671762	1.342884	2.238740	6	–0.283451	3.182270	–0.210893
1	–2.962873	2.695740	3.836442	1	–0.206663	2.994809	–1.287839

1	–0.539879	2.228965	0.257767
6	–1.338749	4.250367	0.062695
1	–1.478908	4.358626	1.145952
1	–2.303474	3.927901	–0.341973
6	–0.936359	5.595861	–0.542252
1	–1.686551	6.356880	–0.308662
1	–0.910392	5.504064	–1.635675
6	0.439118	6.038152	–0.040085
1	0.384993	6.233927	1.038491
1	0.732905	6.979906	–0.511470
6	1.505246	4.975756	–0.310267
1	2.473328	5.278975	0.096828
1	1.637839	4.840709	–1.389788

4–3NAI1a

SCF energy = –2683.02302889

7	–2.209473	–2.304797	–1.146702
15	2.477546	0.034961	–0.096570
6	–1.601745	–2.519009	–2.463934
1	–2.278240	–3.171094	–3.021554
6	–0.281719	–3.275617	–2.313802
1	0.420485	–2.676481	–1.729129
1	0.177497	–3.487680	–3.285358
1	–0.430688	–4.220114	–1.784402
6	–3.485026	–3.007923	–0.919230
1	–3.733723	–2.843810	0.130356
6	–4.607233	–2.375188	–1.746673
1	–5.564142	–2.861645	–1.534807
1	–4.415220	–2.475544	–2.820414
1	–4.705111	–1.315956	–1.505677
79	0.205763	–0.117939	–0.338614
5	–1.840420	–1.278865	–0.215758
7	–1.939059	–1.211973	1.213376
6	–1.721892	–2.259766	2.214330
6	–2.987136	–2.542367	3.033979
1	–3.357598	–1.652256	3.538391
1	–2.787931	–3.311244	3.787460
1	–3.790415	–2.897934	2.384904
6	–0.553228	–1.849813	3.131092
1	–0.727250	–0.908315	3.643472
1	–0.373707	–2.617082	3.890536
1	0.357607	–1.742351	2.531783
6	–1.274888	–3.571913	1.556317
1	–0.948303	–4.274029	2.328720
1	–2.081252	–4.045596	1.004305
1	–0.441073	–3.410420	0.868570
5	–2.614000	0.185680	1.214135
17	–4.549185	–0.073738	1.108534
6	–2.311251	1.326733	2.373030
6	–3.055551	2.649042	2.126936
1	–4.138848	2.509109	2.116097
1	–2.767892	3.117972	1.189245
1	–2.822108	3.365923	2.925018
6	–2.755919	0.890811	3.781091
1	–3.823532	0.656081	3.795290
1	–2.589692	1.706290	4.497199
1	–2.223228	0.023566	4.166847
6	–0.815827	1.672330	2.395740
1	–0.580581	2.385060	3.197708
1	–0.517878	2.143299	1.451947
1	–0.179240	0.795593	2.539730
6	–3.424223	–4.519351	–1.169586
1	–4.319070	–4.995197	–0.759264
1	–3.397224	–4.759408	–2.236525
1	–2.552543	–4.982210	–0.703904
6	–1.437274	–1.265546	–3.319105
1	–1.065570	–1.547425	–4.309640
1	–2.389753	–0.748485	–3.438644
1	–0.738531	–0.544568	–2.888420
6	3.327811	–1.566725	–0.434409
6	3.335504	–1.925581	–1.927725
6	3.955278	–3.304499	–2.169419
6	3.289775	–4.392781	–1.329134
6	3.334859	–4.036317	0.155347
6	2.683095	–2.678878	0.410926
1	4.369801	–1.445633	–0.114467
1	3.902769	–1.180420	–2.492977
1	2.313567	–1.905364	–2.320656
1	3.887929	–3.547881	–3.233992
1	5.025256	–3.264182	–1.925995
1	3.778602	–5.355677	–1.504722
1	2.245023	–4.508358	–1.641320
1	2.825779	–4.800877	0.749442
1	4.378293	–4.015049	0.496830
1	2.733204	–2.434921	1.476811
1	1.617957	–2.743286	0.166519
6	2.616206	1.904886	2.011712
6	2.882351	0.432119	1.668074
6	4.265942	0.007969	2.182430
1	2.134196	–0.161999	2.209505
6	2.694881	2.128238	3.521104
1	1.642537	2.221797	1.635582
1	3.370097	2.532858	1.523139

6	4.053179	1.692920	4.069284
1	2.510443	3.182723	3.746277
1	1.893605	1.560539	4.009374
6	4.364966	0.245076	3.692900
1	4.083355	1.814591	5.156072
1	4.833392	2.348830	3.660944
1	5.363486	–0.034001	4.043057
1	3.658019	–0.422085	4.202430
1	4.458097	–1.047869	1.978556
1	5.049910	0.575756	1.668817
6	3.229346	1.252971	–1.257421
1	3.083356	0.756260	–2.226062
6	2.453745	2.577937	–1.342274
1	2.512914	3.116040	–0.392390
1	1.393832	2.378272	–1.523092
6	3.022578	3.462879	–2.452103
1	2.851693	2.981160	–3.423285
1	2.481289	4.413186	–2.476795
6	4.519938	3.706046	–2.261897
1	4.912838	4.318882	–3.078485
1	4.679207	4.276936	–1.337828
6	5.287929	2.386881	–2.174862
1	5.215015	1.860216	–3.135110
1	6.352007	2.573212	–2.001011
6	4.732562	1.489289	–1.066243
1	4.905324	1.971350	–0.097505
1	5.277077	0.539529	–1.045919
6	–2.039193	0.391542	–0.399150
7	–1.987144	1.106556	–1.452061
6	–2.651994	2.370550	–1.714986
1	–2.704319	2.422964	–2.812356
6	–1.734563	3.527809	–1.292178
1	–1.525648	3.455374	–0.221603
1	–0.772487	3.414865	–1.803505
6	–2.360749	4.884153	–1.616291
1	–2.404472	5.011268	–2.706087
1	–1.721218	5.687252	–1.235510
6	–3.774306	5.004885	–1.044534
1	–4.205007	5.975703	–1.310325
1	–3.729828	4.971121	0.050871
6	–4.668075	3.871375	–1.551043
1	–4.780516	3.964957	–2.639946
1	–5.672657	3.961340	–1.127094
6	–4.086984	2.499700	–1.204252
1	–4.690028	1.702700	–1.649394
1	–4.136462	2.338429	–0.131063

4–3NAI1

SCF energy = –2354.96347724

7	2.738037	1.916746	–0.155819
15	–2.370345	–0.045030	0.044542
6	2.018894	3.140815	–0.557300
1	2.780867	3.905976	–0.728218
6	1.119087	3.688198	0.550613
1	0.287954	3.009692	0.757089
1	0.705865	4.659988	0.260741
1	1.684336	3.816269	1.477516
6	4.203565	2.017769	–0.248466
1	4.587939	1.041303	0.043288
6	4.688551	2.275141	–1.677674
1	5.779851	2.209027	–1.721768
1	4.408586	3.270314	–2.037988
1	4.274064	1.533536	–2.362019
79	–0.011249	0.361636	0.184403
5	2.070348	0.707245	0.159864
7	2.941704	–0.491105	0.559118
6	3.128216	–0.655873	2.033736
6	4.616356	–0.766787	2.384492
1	5.119506	–1.576769	1.865800
1	4.742801	–0.928926	3.459072
1	5.131351	0.162109	2.124477
6	2.304630	–1.853788	2.523806
1	2.578411	–2.780583	2.028221
1	2.424995	–1.993984	3.602635
1	1.246962	–1.666134	2.318490
6	2.606327	0.569169	2.809979
1	2.793027	0.410302	3.875658
1	3.109340	1.488890	2.513999
1	1.533478	0.716961	2.675804
5	3.284931	–1.374043	–0.466888
17	2.632861	–0.794926	–2.104675
6	4.222005	–2.690328	–0.631083
6	3.827309	–3.521171	–1.872769
1	3.951430	–2.971919	–2.805414
1	2.786432	–3.855116	–1.822439
1	4.459475	–4.414838	–1.929380
6	5.647397	–2.143711	–0.883230
1	5.663244	–1.452012	–1.731146
1	6.332588	–2.967293	–1.117783
1	6.053161	–1.612525	–0.018505
6	4.272433	–3.713365	0.518344
1	5.000640	–4.494061	0.270304
1	3.307079	–4.211622	0.648216

1	4.568708	–3.306010	1.482483
6	4.791967	3.044005	0.723695
1	5.884921	3.012181	0.684726
1	4.490745	4.068101	0.483504
1	4.488217	2.840582	1.752738
6	1.272457	2.978643	–1.882131
1	0.830691	3.931273	–2.193422
1	1.950796	2.638428	–2.667300
1	0.473802	2.238461	–1.795067
6	–3.323225	1.540530	0.126940
6	–2.860306	2.478535	–1.002612
6	–3.553160	3.839564	–0.935055
6	–3.340642	4.499947	0.425199
6	–3.824398	3.586235	1.549057
6	–3.140654	2.219126	1.494184
1	–4.389840	1.321613	–0.012306
1	–3.036212	2.022777	–1.981381
1	–1.776680	2.625511	–0.919979
1	–3.175202	4.482109	–1.736177
1	–4.628943	3.713122	–1.115358
1	–3.856856	5.463880	0.468258
1	–2.271534	4.706746	0.562679
1	–3.641787	4.047859	2.524328
1	–4.910931	3.452170	1.464707
1	–3.538823	1.588185	2.293796
1	–2.068216	2.340702	1.692983
6	–2.165990	–2.297899	1.732862
6	–3.065913	–1.098192	1.393925
6	–4.527851	–1.535434	1.255093
1	–2.999955	–0.421585	2.256872
6	–2.651997	–2.992359	3.006482
1	–1.130457	–1.967245	1.851604
1	–2.168766	–3.017735	0.907960
6	–4.118306	–3.412565	2.894926
1	–2.022035	–3.861541	3.218835
1	–2.533812	–2.306809	3.855715
6	–5.012039	–2.225720	2.532863
1	–4.455885	–3.869330	3.830289
1	–4.213947	–4.183446	2.118994
1	–6.049163	–2.553068	2.409372
1	–5.008361	–1.500711	3.357080
1	–5.172448	–0.683045	1.017598
1	–4.615526	–2.240099	0.420322
6	–2.767549	–0.746221	–1.620506
1	–2.165615	–0.098197	–2.273346
6	–2.201990	–2.164987	–1.781859
1	–2.778229	–2.858980	–1.158060
1	–1.165109	–2.203573	–1.433197
6	–2.290668	–2.621808	–3.237959
1	–1.639638	–1.987659	–3.852249
1	–1.907741	–3.642519	–3.331675
6	–3.726332	–2.540394	–3.757408
1	–3.767423	–2.829832	–4.811971
1	–4.348810	–3.261629	–3.211220
6	–4.307357	–1.137912	–3.572803
1	–3.755522	–0.431399	–4.206211
1	–5.348921	–1.109263	–3.908239
6	–4.218425	–0.677030	–2.114751
1	–4.857798	–1.315348	–1.497033
1	–4.614805	0.338370	–2.025337

4–3NAI2

SCF energy = –2683.04120373

7	2.685428	–1.131531	1.805417
15	–2.457868	–0.431133	–0.076656
6	2.050236	–1.058003	3.133099
1	2.847697	–1.191843	3.869165
6	1.057003	–2.193426	3.379514
1	0.189982	–2.108017	2.721200
1	0.709200	–2.178360	4.418029
1	1.529650	–3.160303	3.188851
6	4.150834	–1.250282	1.838938
1	4.454591	–1.251296	0.794644
6	4.818725	–0.040606	2.496740
1	5.903831	–0.093574	2.369957
1	4.617185	0.021995	3.570914
1	4.471221	0.886860	2.034123
79	–0.110074	–0.715635	0.334254
5	1.966061	–1.048604	0.581090
7	2.769418	–1.102111	–0.697422
6	2.857021	–2.420234	–1.379057
6	4.313586	–2.888110	–1.525706
1	4.908474	–2.211940	–2.135686
1	4.350395	–3.874126	–2.000032
1	4.794469	–2.971649	–0.547045
6	2.167960	–2.389288	–2.749452
1	2.603113	–1.650556	–3.420531
1	2.236026	–3.370950	–3.230260
1	1.114317	–2.130300	–2.630689
6	2.140617	–3.503110	–0.549818
1	2.257145	–4.472394	–1.042338
1	2.555675	–3.589602	0.456794
1	1.071302	–3.301449	–0.454549

5	2.972481	0.204360	–1.300932	6	–3.937741	–2.594146	–4.029689
17	1.281821	0.852109	–2.515761	1	–1.822183	–2.581217	–4.510461
6	4.298734	0.778515	–2.087347	1	–2.247409	–3.610083	–3.152021
6	4.243246	2.309441	–2.273676	6	–4.852031	–2.612281	–2.803581
1	4.253538	2.847063	–1.319093	1	–4.181097	–3.428521	–4.694891
1	3.353082	2.615332	–2.827224	1	–4.123368	–1.675171	–4.601138
1	5.122970	2.650592	–2.831476	1	–5.900537	–2.528568	–3.107163
6	5.537873	0.480877	–1.222587	1	–4.750855	–3.576637	–2.288722
1	5.451470	0.932510	–0.227327	1	–5.155374	–1.524979	–0.952637
1	6.439801	0.897792	–1.687341	1	–4.689190	–0.522924	–2.321032
1	5.702761	–0.587198	–1.077254	6	–2.982033	1.314452	–0.412200
6	4.493282	0.189134	–3.491933	1	–2.432404	1.860103	0.366310
1	5.381965	0.629173	–3.961166	6	–2.454206	1.820800	–1.762378
1	3.634376	0.411792	–4.129669	1	–2.991535	1.314161	–2.572415
1	4.637399	–0.891032	–3.491888	1	–1.396050	1.571886	–1.886666
6	4.628722	–2.562519	2.461484	6	–2.677571	3.326484	–1.908175
1	5.714332	–2.655610	2.361375	1	–2.079352	3.857908	–1.157639
1	4.393393	–2.633528	3.528297	1	–2.314587	3.659718	–2.884826
1	4.172126	–3.419294	1.960710	6	–4.150510	3.691418	–1.726780
6	1.435022	0.313315	3.417429	1	–4.288250	4.775269	–1.793329
1	1.069434	0.368088	4.447995	1	–4.733094	3.252919	–2.547523
1	2.179777	1.101763	3.276174	6	–4.689517	3.169040	–0.395416
1	0.597446	0.504804	2.743581	1	–4.184710	3.689246	0.430138
6	–3.434586	–0.909926	1.421246	1	–5.755597	3.397333	–0.297530
6	–3.020030	–0.010234	2.599519	6	–4.467449	1.661222	–0.244145
6	–3.733188	–0.397284	3.894981	1	–5.063454	1.132812	–0.994808
6	–3.492660	–1.866239	4.237057	1	–4.841023	1.339229	0.731705
6	–3.928741	–2.765897	3.082533	6	2.538088	1.335103	–0.214941
6	–3.224608	–2.389986	1.777410	7	2.228943	2.220080	0.455276
1	–4.500965	–0.754664	1.216399	6	1.510503	3.299094	1.058838
1	–3.215913	1.042417	2.371536	1	1.776997	3.307319	2.120922
1	–1.936025	–0.100541	2.745128	6	0.010082	3.032962	0.900285
1	–3.390598	0.248372	4.709778	1	–0.194525	2.884855	–0.165308
1	–4.811366	–0.220093	3.786209	1	–0.245800	2.096106	1.400551
1	–4.024155	–2.137590	5.154472	6	–0.801401	4.202241	1.452736
1	–2.423804	–2.021462	4.432661	1	–0.660622	4.267021	2.539146
1	–3.727255	–3.815737	3.316650	1	–1.866811	4.011488	1.291847
1	–5.014807	–2.678538	2.946462	6	–0.392403	5.525341	0.804900
1	–3.593504	–3.033598	0.973820	1	–0.961164	6.352366	1.239528
1	–2.149779	–2.588888	1.871814	1	–0.641079	5.498664	–0.263261
6	–2.109259	–1.516989	–2.655082	6	1.107881	5.776303	0.964398
6	–3.026259	–1.562085	–1.420514	1	1.343851	5.913469	2.027450
6	–4.500483	–1.484387	–1.829454	1	1.396401	6.702913	0.461102
1	–2.858088	–2.545109	–0.958473	6	1.931913	4.617580	0.402980
6	–2.463170	–2.643589	–3.626152	1	3.001084	4.783840	0.559337
1	–1.061157	–1.585805	–2.353660	1	1.772828	4.526823	–0.677044
1	–2.209047	–0.556598	–3.168690				

4–3NAI3

SCF energy = –2683.04553325

7	2.762828	0.599287	1.737423
15	–2.310660	–0.415445	0.345786
6	2.043071	1.365621	2.760722
1	2.809999	1.833918	3.381505
6	1.244595	0.439612	3.679752
1	0.556701	–0.179692	3.097707
1	0.660996	1.011132	4.409043
1	1.908353	–0.234224	4.226158
6	4.231366	0.669665	1.829571
1	4.602266	–0.001668	1.057739
6	4.734281	2.071791	1.478561
1	5.826986	2.090628	1.434677
1	4.420955	2.816549	2.217742
1	4.348880	2.376781	0.503001
79	–0.020757	–0.022378	0.158243
5	2.219721	–0.125683	0.629009
7	2.646845	–1.342060	0.025962
6	2.984679	–2.612778	0.680444
6	4.494545	–2.767513	0.921203
1	5.053793	–2.681832	–0.010116
1	4.710377	–3.749724	1.352559
1	4.872888	–2.015403	1.614086
6	2.501657	–3.791886	–0.172983
1	2.963581	–3.799467	–1.159592
1	2.749543	–4.732408	0.328708
1	1.421947	–3.750576	–0.322022
6	2.261541	–2.694119	2.031568
1	2.459017	–3.655877	2.513122
1	2.581447	–1.902587	2.709246
1	1.179689	–2.598044	1.891344
5	2.554398	–0.901653	–1.429370
17	1.068512	–1.845903	–2.382975
6	3.851352	–0.813609	–2.416686
6	3.497994	–0.068441	–3.715660
1	3.141734	0.943080	–3.516332
1	2.716766	–0.592546	–4.271801
1	4.381926	0.000351	–4.363578
6	4.980794	–0.038056	–1.720963
1	4.650044	0.956537	–1.405451
1	5.829473	0.102331	–2.401946
1	5.356910	–0.564642	–0.839241
6	4.386826	–2.195027	–2.824089
1	5.217151	–2.085384	–3.533618
1	3.612743	–2.792672	–3.313154
1	4.767353	–2.769627	–1.976329
6	4.792349	0.189818	3.169878
1	5.880156	0.096425	3.106470
1	4.576233	0.884980	3.986589
1	4.386791	–0.786427	3.443036
6	1.182443	2.519771	2.247365
1	0.898668	3.167347	3.083030
1	1.729615	3.120505	1.518997
1	0.262284	2.164645	1.780766
6	–3.128336	0.652129	1.610927
6	–2.949823	2.131786	1.225924
6	–3.512732	3.077940	2.285627
6	–2.905642	2.798899	3.658360
6	–3.135924	1.343521	4.058687
6	–2.566106	0.382759	3.014559
1	–4.199392	0.413475	1.609820
1	–3.423737	2.340211	0.263248
1	–1.880997	2.338348	1.091711
1	–3.325230	4.112993	1.984231
1	–4.602776	2.959689	2.339737
1	–3.328139	3.474240	4.408201
1	–1.826728	2.998643	3.624169
1	–2.676163	1.135523	5.029642
1	–4.212254	1.163806	4.177487
1	–2.767421	–0.648071	3.319682
1	–1.477799	0.496914	2.988192
6	–1.704924	–3.156353	0.122200
6	–2.649049	–2.162424	0.820734
6	–4.107295	–2.622865	0.715475
1	–2.369373	–2.167159	1.883694
6	–1.875807	–4.557373	0.708610
1	–0.666395	–2.831769	0.222071
1	–1.904674	–3.180613	–0.953401
6	–3.329505	–5.026617	0.639682
1	–1.222621	–5.255485	0.177464
1	–1.541668	–4.552720	1.754616
6	–4.273030	–4.024971	1.307235
1	–3.434815	–6.011087	1.105473
1	–3.618348	–5.147139	–0.412428
1	–5.312436	–4.350491	1.200683
1	–4.065193	–3.987874	2.384535
1	–4.781646	–1.919711	1.215589
1	–4.400817	–2.649183	–0.339896
6	–3.112054	0.043402	–1.252991
1	–2.679472	1.037131	–1.434106
6	–2.651348	–0.855468	–2.410157
1	–3.081707	–1.856393	–2.284132

1	–1.564794	–0.976548	–2.407787
6	–3.114910	–0.280450	–3.748362
1	–2.611123	0.679825	–3.917909
1	–2.799506	–0.942483	–4.559319
6	–4.629787	–0.077044	–3.776930
1	–4.935870	0.379210	–4.723150
1	–5.126574	–1.054869	–3.726756
6	–5.097374	0.783119	–2.602234
1	–4.690641	1.797317	–2.711203
1	–6.187346	0.881925	–2.609271
6	–4.638706	0.205189	–1.260065
1	–5.120150	–0.764535	–1.101858
1	–4.975198	0.857180	–0.449133
6	1.837927	0.543001	–1.056232
7	1.765899	1.633127	–1.666060
6	0.873241	2.705723	–1.305112
1	0.428042	2.510526	–0.317281
6	–0.274230	2.746411	–2.319807
1	0.145977	2.900188	–3.320161
1	–0.766291	1.768265	–2.338809
6	–1.260931	3.860001	–1.976744
1	–1.739727	3.637136	–1.013812
1	–2.061640	3.897594	–2.722787
6	–0.554705	5.214561	–1.884214
1	–1.264047	5.993481	–1.586903
1	–0.182642	5.492069	–2.878545
6	0.621704	5.167599	–0.905808
1	0.239112	5.006379	0.111419
1	1.141070	6.130516	–0.892256
6	1.600629	4.045428	–1.256858
1	2.413573	3.996714	–0.525139
1	2.065071	4.231979	–2.231966

4–3NAI4

SCF energy = –2683.06322122

7	–3.164264	–1.545081	–1.225843
15	2.543866	–0.550258	0.070577
6	–2.633771	–1.775935	–2.584896
1	–3.365381	–2.413706	–3.085393
6	–1.326004	–2.571574	–2.551840
1	–0.541975	–2.008833	–2.037221
1	–0.977619	–2.778149	–3.568939
1	–1.454794	–3.526497	–2.035040
6	–4.385448	–2.303352	–0.922616
1	–4.660945	–2.009928	0.088457
6	–5.549346	–1.892468	–1.834078
1	–6.488201	–2.294594	–1.442490
1	–5.435251	–2.274630	–2.852507
1	–5.638644	–0.807111	–1.887652
79	0.340043	0.033255	–0.465800
5	–2.627252	–0.596303	–0.316832
7	–2.809218	–0.605082	1.176277
6	–2.387684	–1.782930	2.012779
6	–3.629217	–2.583216	2.445173
1	–4.355719	–1.921338	2.923659
1	–3.352000	–3.356055	3.168651
1	–4.121174	–3.081753	1.612323
6	–1.653585	–1.397020	3.304871
1	–2.279781	–0.833024	3.996878
1	–1.352141	–2.317995	3.812214
1	–0.756896	–0.814462	3.101761
6	–1.417710	–2.690699	1.245520
1	–1.204868	–3.587592	1.834168
1	–1.803770	–3.004842	0.279839
1	–0.471591	–2.170339	1.069558
5	–3.060410	0.723964	1.663204
17	–1.923421	1.582747	2.810606
6	–4.387154	1.558356	1.352765
6	–4.194886	3.067224	1.161002
1	–3.647092	3.257100	0.236512
1	–3.653374	3.529170	1.989086
1	–5.171357	3.560810	1.083643
6	–5.167453	1.021564	0.149566
1	–4.592969	1.137732	–0.773449
1	–6.105147	1.577106	0.029585
1	–5.428963	–0.029995	0.279341
6	–5.248032	1.319067	2.620507
1	–6.228841	1.790683	2.489746
1	–4.790175	1.746597	3.516544
1	–5.424238	0.252715	2.802917
6	–4.210111	–3.824494	–0.950184
1	–5.138126	–4.311319	–0.636145
1	–3.980001	–4.189287	–1.955519
1	–3.416467	–4.162077	–0.281998
6	–2.503445	–0.529023	–3.462243
1	–2.452983	–0.832577	–4.513130
1	–3.357936	0.136667	–3.330090
1	–1.603475	0.042075	–3.233912
6	3.074361	–2.119154	–0.747383
6	2.995150	–1.946821	–2.275129
6	3.329168	–3.241152	–3.017130
6	2.434497	–4.390734	–2.559261
6	2.540972	–4.585442	–1.048498

6	2.199067	–3.299621	–0.294193
1	4.115025	–2.327275	–0.468031
1	3.666744	–1.150474	–2.609024
1	1.979527	–1.629786	–2.543829
1	3.225435	–3.079907	–4.094392
1	4.380324	–3.503329	–2.838861
1	2.699996	–5.314168	–3.082769
1	1.392531	–4.166340	–2.821440
1	1.874516	–5.387647	–0.717281
1	3.561459	–4.899710	–0.793046
1	2.308672	–3.471206	0.780379
1	1.144591	–3.053337	–0.467698
6	1.983105	0.224101	2.724168
6	2.726437	–0.829729	1.884745
6	4.150924	–1.036594	2.410060
1	2.174031	–1.769921	2.022067
6	1.960541	–0.185938	4.196397
1	0.963888	0.362465	2.353339
1	2.475575	1.197205	2.630183
6	3.373029	–0.414966	4.735101
1	1.441922	0.578264	4.782389
1	1.375322	–1.108193	4.303682
6	4.132102	–1.437682	3.887768
1	3.334313	–0.743414	5.778193
1	3.920510	0.536590	4.727726
1	5.156759	–1.552832	4.254943
1	3.652277	–2.419948	3.987680
1	4.684155	–1.789912	1.820851
1	4.709873	–0.099521	2.306075
6	3.710512	0.743499	–0.542052
1	3.352117	0.880726	–1.572221
6	3.498683	2.086344	0.173829
1	3.871548	2.011659	1.202023
1	2.432548	2.325829	0.239198
6	4.253377	3.203499	–0.545993
1	3.822509	3.339781	–1.546174
1	4.110242	4.149913	–0.016212
6	5.742287	2.875782	–0.666638
1	6.260966	3.661230	–1.224642
1	6.189425	2.859154	0.335956
6	5.965115	1.518283	–1.335963
1	5.627324	1.568581	–2.379297
1	7.033114	1.280897	–1.366265
6	5.203294	0.399197	–0.618666
1	5.613486	0.270840	0.388119
1	5.363285	–0.547738	–1.142276
6	–1.641503	0.546597	–0.788161
7	–2.070558	1.707804	–1.107140
6	–1.101545	2.746462	–1.439475
1	–0.218403	2.279456	–1.914954
6	–0.608036	3.485673	–0.192399
1	–1.465354	3.919655	0.334295
1	–0.157895	2.765842	0.499365
6	0.390827	4.581981	–0.561761
1	1.289351	4.122267	–0.997357
1	0.718516	5.112260	0.338811
6	–0.207754	5.563269	–1.571164
1	0.531906	6.319411	–1.854895
1	–1.039881	6.099480	–1.096831
6	–0.725690	4.832532	–2.811704
1	0.124762	4.391420	–3.349263
1	–1.193631	5.541575	–3.502389
6	–1.713693	3.726705	–2.437300
1	–2.042063	3.180312	–3.327512
1	–2.614355	4.164008	–1.988828

4–3NATS1

SCF energy = –2354.94328183

7	2.927713	1.785269	–0.173110
15	–2.284577	0.104842	–0.011718
6	2.280612	3.083171	–0.458103
1	3.087689	3.814375	–0.547976
6	1.409156	3.573611	0.698249
1	0.530977	2.937984	0.827912
1	1.070455	4.598245	0.512081
1	1.972032	3.563701	1.635375
6	4.396656	1.845067	–0.181944
1	4.718387	0.819299	–0.025126
6	4.952740	2.294815	–1.537380
1	6.030720	2.114340	–1.578774
1	4.794530	3.361551	–1.722543
1	4.486213	1.742544	–2.355445
79	0.099643	0.385528	–0.086018
5	2.200101	0.584110	0.051642
7	2.964809	–0.655512	0.500885
6	3.285414	–0.839796	1.952938
6	4.808440	–0.827689	2.159413
1	5.281757	–1.619509	1.571894
1	5.058266	–0.998598	3.211743
1	5.252289	0.123151	1.863102
6	2.757604	–2.177476	2.492460
1	3.197261	–3.035275	1.973259
1	3.016356	–2.273084	3.550769

1	1.673533	–2.247410	2.395606
6	2.643938	0.266340	2.799456
1	2.922205	0.136093	3.849092
1	2.959569	1.261331	2.487151
1	1.554050	0.228144	2.725279
5	2.802756	–1.785271	–0.360469
17	1.271382	–2.822725	–0.282428
6	3.839971	–2.320268	–1.451228
6	3.172635	–2.564508	–2.816019
1	2.712158	–1.650411	–3.205853
1	2.396856	–3.330112	–2.763033
1	3.921646	–2.893719	–3.545812
6	5.002069	–1.341975	–1.651153
1	4.651813	–0.389660	–2.053120
1	5.729799	–1.752024	–2.361369
1	5.527575	–1.133768	–0.716658
6	4.410428	–3.655385	–0.923617
1	5.155468	–4.043017	–1.628221
1	3.633010	–4.413700	–0.804777
1	4.912989	–3.532615	0.042445
6	4.979314	2.705352	0.942405
1	6.070944	2.627744	0.946807
1	4.731105	3.764421	0.823429
1	4.618988	2.386481	1.921932
6	1.539411	3.110848	–1.794709
1	1.171708	4.121010	–2.003353
1	2.203732	2.812468	–2.609189
1	0.688705	2.426846	–1.790341
6	–3.176147	1.726178	–0.048336
6	–2.805681	2.473483	–1.341057
6	–3.450289	3.857488	–1.410760
6	–3.084736	4.695769	–0.187634
6	–3.477695	3.972074	1.098328
6	–2.843280	2.582308	1.183565
1	–4.256484	1.534339	–0.049250
1	–3.092297	1.889392	–2.220976
1	–1.715189	2.583060	–1.384941
1	–3.136321	4.361836	–2.329780
1	–4.541694	3.751204	–1.468380
1	–3.568713	5.676060	–0.236283
1	–2.002045	4.876751	–0.184954
1	–3.185308	4.560211	1.973864
1	–4.570604	3.873882	1.139160
1	–3.186493	2.088459	2.097177
1	–1.754613	2.683857	1.269904
6	–1.929595	–1.900487	1.952266
6	–2.794051	–0.683714	1.579469
6	–4.283650	–0.992249	1.760658
1	–2.524747	0.101252	2.299831
6	–2.223011	–2.346301	3.385360
1	–0.869122	–1.661217	1.835120
1	–2.129973	–2.732476	1.270533
6	–3.710425	–2.636325	3.592551
1	–1.626166	–3.231362	3.626231
1	–1.905589	–1.557993	4.080496
6	–4.573522	–1.437589	3.196257
1	–3.902762	–2.911932	4.634132
1	–3.996985	–3.502987	2.982319
1	–5.635650	–1.678349	3.306362
1	–4.370497	–0.602284	3.879281
1	–4.898365	–0.122972	1.504481
1	–4.572886	–1.796381	1.073955
6	–2.957899	–0.821444	–1.466601
1	–2.426012	–0.338477	–2.298846
6	–2.508653	–2.289697	–1.452093
1	–3.030193	–2.818318	–0.645404
1	–1.438170	–2.362620	–1.240980
6	–2.840052	–2.975653	–2.776887
1	–2.256889	–2.508929	–3.580749
1	–2.531613	–4.024691	–2.737075
6	–4.331227	–2.869488	–3.096334
1	–4.547131	–3.326563	–4.066984
1	–4.900959	–3.438962	–2.350055
6	–4.799286	–1.413675	–3.082190
1	–4.315386	–0.871092	–3.904892
1	–5.877198	–1.356771	–3.264246
6	–4.460928	–0.718128	–1.759735
1	–5.033328	–1.182548	–0.950274
1	–4.781576	0.326323	–1.808422

4–3NATS2

SCF energy = –2683.02225906

7	2.758183	–0.351148	1.950892
15	–2.384960	–0.607357	0.001835
6	2.082102	0.027399	3.204228
1	2.867146	0.148193	3.955668
6	1.161710	–1.071093	3.735496
1	0.315322	–1.228945	3.064099
1	0.776702	–0.804507	4.725683
1	1.703207	–2.016806	3.820681
6	4.226255	–0.342183	2.035444
1	4.564464	–0.603470	1.036322
6	4.787146	1.047500	2.346372

1	5.877209	1.041803	2.252682	6	–3.012665	–1.722111	2.490360
1	4.548833	1.380170	3.362288	1	–4.411161	–0.541409	1.365484
1	4.392561	1.784357	1.643987	1	–3.311321	1.656514	1.686251
79	–0.017721	–0.537280	0.416059	1	–1.921430	0.875674	2.426909
5	2.074441	–0.631909	0.733025	1	–3.384240	1.841623	4.154612
7	2.921563	–1.103398	–0.435548	1	–4.765940	0.938980	3.549560
6	3.103829	–2.582838	–0.575084	1	–3.799177	–0.215638	5.526173
6	4.587759	–2.976539	–0.513837	1	–2.223188	–0.272546	4.745282
1	5.165370	–2.523565	–1.318294	1	–3.380931	–2.454048	4.485143
1	4.699981	–4.062235	–0.601099	1	–4.763677	–1.656396	3.750757
1	5.034221	–2.669419	0.434446	1	–3.338396	–2.652342	2.015652
6	2.490439	–3.090976	–1.889104	1	–1.925714	–1.796672	2.615000
1	2.952038	–2.636942	–2.768164	6	–2.007067	–2.566182	–1.992211
1	2.614586	–4.175186	–1.973928	6	–2.849091	–2.227403	–0.751161
1	1.423499	–2.859534	–1.922803	6	–4.334437	–2.494202	–1.012247
6	2.390904	–3.337594	0.559691	1	–2.516646	–2.922360	0.033248
1	2.571310	–4.410078	0.444615	6	–2.223471	–4.023910	–2.400505
1	2.752927	–3.039372	1.543969	1	–0.947896	–2.374559	–1.798670
1	1.311550	–3.171624	0.537418	1	–2.290631	–1.916776	–2.826690
5	3.022967	–0.227846	–1.572933	6	–3.704354	–4.326591	–2.636544
17	1.459605	0.072682	–2.595311	1	–1.642189	–4.246699	–3.300358
6	4.346673	0.284045	–2.340909	1	–1.837408	–4.680074	–1.609707
6	4.164855	1.648521	–3.031752	6	–4.554715	–3.953058	–1.420905
1	3.929991	2.438695	–2.315262	1	–3.842680	–5.384148	–2.881993
1	3.370678	1.626629	–3.780020	1	–4.053425	–3.756322	–3.507429
1	5.095511	1.929781	–3.539162	1	–5.615171	–4.126947	–1.629421
6	5.525979	0.412280	–1.365241	1	–4.291033	–4.605522	–0.578204
1	5.307329	1.146962	–0.585412	1	–4.938748	–2.253925	–0.131395
1	6.426168	0.747100	–1.894647	1	–4.683344	–1.842719	–1.821276
1	5.764876	–0.530047	–0.870826	6	–3.030040	0.821802	–0.978534
6	4.714982	–0.714123	–3.461854	1	–2.619780	1.659749	–0.402417
1	5.593369	–0.346146	–4.004559	6	–2.391824	0.914123	–2.370829
1	3.901116	–0.820396	–4.185073	1	–2.785078	0.115567	–3.009852
1	4.964926	–1.708951	–3.089732	1	–1.310816	0.761812	–2.307159
6	4.779056	–1.387719	3.006483	6	–2.710617	2.260197	–3.022398
1	5.870552	–1.426285	2.936729	1	–2.245798	3.064848	–2.437873
1	4.529648	–1.166566	4.049237	1	–2.263990	2.304647	–4.019938
1	4.394462	–2.383644	2.776185	6	–4.218548	2.500246	–3.096469
6	1.370837	1.378771	3.119364	1	–4.427921	3.484546	–3.526813
1	0.961791	1.660209	4.095413	1	–4.666861	1.762080	–3.774339
1	2.068241	2.156767	2.799075	6	–4.868836	2.375686	–1.718562
1	0.551783	1.337364	2.398992	1	–4.508717	3.188295	–1.073543
6	–3.337068	–0.520708	1.588332	1	–5.953374	2.501364	–1.796955
6	–3.009205	0.802954	2.301694	6	–4.547082	1.032071	–1.056663
6	–3.675519	0.902693	3.673410	1	–5.006977	0.226871	–1.638376
6	–3.303814	–0.288947	4.553113	1	–5.001674	0.997841	–0.062368
6	–3.672892	–1.601056	3.864731	6	2.571297	1.895378	–0.324951

7	1.895848	2.791237	–0.017448
6	0.911237	3.770722	0.306435
1	1.056107	4.028879	1.361998
6	–0.483243	3.166729	0.122937
1	–0.561115	2.798634	–0.905990
1	–0.586382	2.293984	0.770960
6	–1.564574	4.204598	0.412786
1	–1.532147	4.476055	1.475793
1	–2.551964	3.765087	0.240721
6	–1.386432	5.458820	–0.442423
1	–2.147672	6.202456	–0.188872
1	–1.538173	5.201952	–1.498537
6	0.011897	6.052239	–0.263858
1	0.123307	6.418047	0.764999
1	0.144979	6.919739	–0.916136
6	1.101465	5.020681	–0.558003
1	2.095623	5.441306	–0.384734
1	1.058733	4.718722	–1.610644

4–3NATS3

SCF energy = –2683.03500571

7	2.794668	–0.322666	1.958209
15	–2.354251	–0.508434	0.117813
6	2.142557	0.173060	3.180261
1	2.927686	0.259633	3.935803
6	1.129933	–0.825958	3.738710
1	0.288025	–0.948824	3.053086
1	0.739638	–0.485415	4.703474
1	1.594143	–1.805151	3.879275
6	4.257404	–0.433908	2.043830
1	4.569322	–0.767269	1.057105
6	4.917502	0.926895	2.279468
1	6.002827	0.841868	2.175617
1	4.713836	1.324677	3.278773
1	4.564764	1.653061	1.544023
79	0.007261	–0.287257	0.391394
5	2.127306	–0.576280	0.728469
7	2.700959	–1.246208	–0.437847
6	2.986697	–2.695732	–0.461522
6	4.485296	–3.017711	–0.308873
1	5.087423	–2.469400	–1.033192
1	4.663751	–4.085965	–0.466842
1	4.854999	–2.773706	0.688233
6	2.481163	–3.340419	–1.759438
1	2.959520	–2.926480	–2.646202
1	2.685379	–4.415518	–1.735712
1	1.406636	–3.194914	–1.872805
6	2.234886	–3.384625	0.690282
1	2.442919	–4.458401	0.689886
1	2.524077	–2.984985	1.663850
1	1.154758	–3.245010	0.580185
5	2.595997	–0.256587	–1.556442
17	1.115532	–0.622003	–2.863806
6	3.905289	0.271495	–2.406261
6	3.591775	1.497391	–3.281144
1	3.288760	2.363908	–2.688903
1	2.793256	1.283828	–3.995228
1	4.483199	1.787865	–3.851374
6	5.028566	0.660415	–1.434125
1	4.705089	1.435145	–0.731437
1	5.893077	1.058683	–1.979677
1	5.375190	–0.193626	–0.847462
6	4.436775	–0.814899	–3.355796
1	5.296617	–0.431388	–3.919466
1	3.675485	–1.118327	–4.078927
1	4.774858	–1.708228	–2.828570
6	4.731592	–1.465478	3.068157
1	5.813250	–1.607916	2.987352
1	4.521933	–1.156171	4.096919
1	4.252885	–2.433517	2.906733
6	1.543324	1.571818	3.030350
1	1.160878	1.930442	3.991394
1	2.303528	2.275076	2.681282
1	0.719560	1.573388	2.313874
6	–3.245630	–0.372393	1.730970
6	–2.907648	0.979739	2.384238
6	–3.553390	1.129303	3.761151
6	–3.158705	–0.024923	4.680141
6	–3.527111	–1.366795	4.051004
6	–2.895212	–1.537644	2.668646
1	–4.324382	–0.408324	1.534478
1	–3.217553	1.807358	1.738104
1	–1.818185	1.059309	2.490280
1	–3.261129	2.087759	4.201008
1	–4.645652	1.153819	3.653092
1	–3.639506	0.082520	5.657183
1	–2.075499	0.007995	4.855275
1	–3.214880	–2.191697	4.698619
1	–4.619045	–1.437019	3.960563
1	–3.229600	–2.485611	2.237998
1	–1.805805	–1.606851	2.772712
6	–1.889742	–2.597506	–1.726455
6	–2.783006	–2.173555	–0.549285

6	–4.261368	–2.428730	–0.859525
1	–2.498171	–2.822001	0.291116
6	–2.126048	–4.067969	–2.070543
1	–0.836863	–2.426148	–1.491860
1	–2.100088	–1.982570	–2.606341
6	–3.600696	–4.350522	–2.361136
1	–1.506948	–4.345997	–2.928396
1	–1.793151	–4.692910	–1.231214
6	–4.493733	–3.902274	–1.203145
1	–3.752790	–5.415148	–2.563799
1	–3.897054	–3.814127	–3.272047
1	–5.548266	–4.066063	–1.446560
1	–4.278476	–4.515454	–0.318162
1	–4.898634	–2.131197	–0.019780
1	–4.560419	–1.814594	–1.716717
6	–3.062169	0.852537	–0.916310
1	–2.605376	1.737279	–0.455544
6	–2.543204	0.794233	–2.360171
1	–2.991648	–0.065814	–2.870697
1	–1.460427	0.637715	–2.381307
6	–2.919920	2.063466	–3.124162
1	–2.403311	2.923880	–2.678614
1	–2.565018	1.989465	–4.155934
6	–4.428175	2.308426	–3.088632
1	–4.676035	3.241581	–3.603800
1	–4.937252	1.504393	–3.636140
6	–4.948846	2.344263	–1.651484
1	–4.519455	3.212529	–1.133541
1	–6.034589	2.482344	–1.640762
6	–4.580335	1.072174	–0.881637
1	–5.098164	0.217955	–1.328504
1	–4.941591	1.154911	0.147652
6	1.911996	1.034899	–0.770932
7	1.810041	2.222229	–0.748754
6	1.154143	3.353129	–0.153042
1	1.492716	3.414969	0.888198
6	–0.362968	3.155981	–0.173168
1	–0.662374	2.946733	–1.206587
1	–0.610576	2.268768	0.414324
6	–1.103324	4.378659	0.359947
1	–0.890137	4.496554	1.430220
1	–2.183379	4.214490	0.276140
6	–0.695063	5.650038	–0.384072
1	–1.205881	6.519873	0.039698
1	–1.015338	5.574828	–1.431177
6	0.821070	5.846935	–0.333713
1	1.128538	6.018614	0.706220
1	1.109066	6.741833	–0.892588
6	1.560409	4.630624	–0.890232
1	2.643532	4.763110	–0.818556
1	1.326920	4.501642	–1.953424

4–3NATS4

SCF energy = –2683.04065592

7	2.864346	–0.607452	1.767548
15	–2.313176	–0.505583	0.149974
6	2.281261	–0.092160	3.009442
1	3.030307	–0.266406	3.785016
6	1.043337	–0.881566	3.437127
1	0.240819	–0.758126	2.706116
1	0.671510	–0.532443	4.406539
1	1.266671	–1.948496	3.514354
6	4.193020	–1.211706	1.933101
1	4.500469	–1.518393	0.935540
6	5.242060	–0.208598	2.425658
1	6.240295	–0.653868	2.378948
1	5.072503	0.097708	3.462456
1	5.240741	0.685773	1.801227
79	–0.056348	0.057369	0.219168
5	2.373680	–0.463653	0.409060
7	2.611882	–1.287699	–0.728555
6	2.511779	–2.731226	–0.958568
6	3.858708	–3.436716	–0.721595
1	4.657100	–2.941654	–1.278529
1	3.808791	–4.477625	–1.055352
1	4.135246	–3.447475	0.332771
6	2.080831	–3.026491	–2.399686
1	2.801700	–2.635164	–3.120399
1	2.007591	–4.108034	–2.547812
1	1.114214	–2.581904	–2.629807
6	1.463884	–3.319288	–0.003661
1	1.411005	–4.407430	–0.105938
1	1.699166	–3.080705	1.035997
1	0.474285	–2.905782	–0.221291
5	2.695581	–0.078964	–1.572394
17	1.205046	0.127570	–2.804999
6	4.057351	0.526578	–2.192555
6	3.872017	1.893859	–2.867299
1	3.482480	2.629622	–2.161991
1	3.180749	1.836879	–3.711222
1	4.834755	2.259019	–3.248120
6	5.106446	0.680654	–1.083440
1	4.765249	1.384704	–0.319098

1	6.048079	1.066501	–1.492640
1	5.327412	–0.273695	–0.597617
6	4.599954	–0.454426	–3.246421
1	5.521877	–0.062518	–3.694012
1	3.880592	–0.610354	–4.056239
1	4.838171	–1.430481	–2.813351
6	4.175449	–2.461179	2.818313
1	5.152724	–2.952929	2.802954
1	3.950692	–2.222103	3.862450
1	3.429065	–3.179917	2.473400
6	2.018331	1.413337	3.029746
1	1.860522	1.751922	4.058682
1	2.866911	1.957680	2.611481
1	1.128543	1.677849	2.457224
6	–3.090649	–0.727164	1.807661
6	–2.812248	0.510674	2.677875
6	–3.401248	0.358879	4.079950
6	–2.880016	–0.905512	4.760217
6	–3.180436	–2.139731	3.912413
6	–2.610707	–2.012959	2.498124
1	–4.173629	–0.811258	1.655787
1	–3.210535	1.412424	2.201899
1	–1.728559	0.657721	2.756974
1	–3.159036	1.243872	4.676025
1	–4.496330	0.314038	4.014793
1	–3.321760	–1.013581	5.755367
1	–1.795888	–0.817857	4.903004
1	–2.775746	–3.038651	4.386882
1	–4.267485	–2.281004	3.851196
1	–2.907916	–2.890377	1.916802
1	–1.515885	–2.021751	2.541555
6	–1.803240	–2.209501	–2.053986
6	–2.597764	–2.089039	–0.744675
6	–4.060554	–2.495123	–0.951077
1	–2.141503	–2.809131	–0.050853
6	–1.874967	–3.641795	–2.580461
1	–0.765930	–1.906278	–1.902735
1	–2.205431	–1.529959	–2.809833
6	–3.324784	–4.087900	–2.778694
1	–1.321052	–3.715178	–3.520693
1	–1.372631	–4.312748	–1.871322
6	–4.146461	–3.922902	–1.498374
1	–3.362007	–5.127879	–3.116871
1	–3.778173	–3.485193	–3.576446
1	–5.192717	–4.187510	–1.680188
1	–3.775683	–4.620187	–0.735818
1	–4.628603	–2.417317	–0.018032
1	–4.528491	–1.806638	–1.664451
6	–3.213404	0.909313	–0.631077
1	–2.749964	1.772557	–0.132390
6	–2.891687	1.035545	–2.128375
1	–3.366953	0.208232	–2.667514
1	–1.815469	0.952018	–2.307415
6	–3.430717	2.352243	–2.685021
1	–2.909326	3.186772	–2.202289
1	–3.206776	2.420296	–3.753446
6	–4.935158	2.478112	–2.443920
1	–5.301564	3.442027	–2.809841
1	–5.459164	1.705798	–3.022306
6	–5.274470	2.312661	–0.962814
1	–4.844883	3.150463	–0.398213
1	–6.357285	2.357922	–0.810663
6	–4.726745	1.000072	–0.394504
1	–5.232978	0.154078	–0.872517
1	–4.962404	0.944409	0.671642
6	1.906725	0.961099	–0.165504
7	2.047639	2.211880	–0.241211
6	1.002863	3.133814	0.154163
1	0.299915	2.650508	0.857309
6	0.199315	3.527496	–1.092163
1	0.891240	3.932959	–1.839125
1	–0.239081	2.628527	–1.536169
6	–0.877004	4.556078	–0.750554
1	–1.623716	4.096552	–0.086802
1	–1.409212	4.853062	–1.659898
6	–0.281610	5.785627	–0.063747
1	–1.073365	6.489541	0.212328
1	0.370691	6.310205	–0.773348
6	0.533251	5.390981	1.168643
1	–0.139970	4.967637	1.926412
1	0.990561	6.276016	1.621526
6	1.612108	4.365250	0.819792
1	2.161800	4.064843	1.716311
1	2.343641	4.803009	0.130581

4–3NATS5

SCF energy = –2683.03681737

7	–3.149305	–0.755960	–1.803694
15	2.823528	–0.246433	–0.094478
6	–2.959549	–0.022565	–3.049772
1	–3.061273	–0.756039	–3.854048
6	–1.566533	0.596865	–3.276742
1	–1.375731	1.480660	–2.667475

1	–1.455990	0.892171	–4.325814	6	2.917768	–2.059020	–0.439489
1	–0.786471	–0.132152	–3.044980	6	2.250717	–2.345055	–1.798083
6	–3.142223	–2.212381	–1.937349	6	2.173821	–3.841005	–2.101329
1	–3.373156	–2.598830	–0.943761	6	1.469429	–4.596222	–0.976799
6	–4.205639	–2.762863	–2.897620	6	2.174407	–4.357202	0.355550
1	–4.310814	–3.842712	–2.757249	6	2.253175	–2.867118	0.688432
1	–3.947226	–2.604145	–3.949511	1	3.975476	–2.345048	–0.497350
1	–5.180592	–2.302980	–2.724659	1	2.783058	–1.829741	–2.604455
79	0.578563	0.368250	–0.074882	1	1.233356	–1.936719	–1.787938
5	–2.950829	–0.196908	–0.448153	1	1.649240	–3.988594	–3.050192
7	–3.570978	–0.790304	0.756620	1	3.187167	–4.243373	–2.235113
6	–4.994421	–0.896523	1.089438	1	1.433663	–5.666658	–1.201240
6	–5.844195	–0.729525	–0.173809	1	0.431682	–4.253063	–0.899675
1	–5.653962	0.230950	–0.660414	1	1.647857	–4.873659	1.163244
1	–6.906165	–0.774464	0.085121	1	3.187338	–4.780646	0.314618
1	–5.635397	–1.514029	–0.897946	1	2.805091	–2.739712	1.624429
6	–5.443383	0.194838	2.075841	1	1.239081	–2.491328	0.864517
1	–5.237450	1.185707	1.662486	6	3.315099	1.358794	2.194212
1	–6.519233	0.124434	2.266438	6	3.585877	–0.018329	1.567206
1	–4.935004	0.118032	3.036755	6	5.065860	–0.397659	1.679808
6	–5.274249	–2.283251	1.682308	1	3.006089	–0.734849	2.164254
1	–6.336404	–2.404923	1.917515	6	3.770474	1.373793	3.655042
1	–4.984867	–3.061697	0.971977	1	2.249414	1.598072	2.128687
1	–4.706612	–2.449993	2.601078	1	3.847231	2.140707	1.642908
5	–2.391416	–1.110573	1.498813	6	5.241699	0.978494	3.790715
17	–1.568291	–2.773663	1.120927	1	3.602470	2.365823	4.084957
6	–1.838433	–0.511944	2.902475	1	3.148789	0.676048	4.230176
6	–0.345177	–0.765503	3.175417	6	5.518345	–0.377833	3.141500
1	0.293373	–0.323495	2.404251	1	5.532294	0.958580	4.845412
1	–0.111998	–1.830489	3.227295	1	5.866996	1.741975	3.309309
1	–0.062281	–0.309545	4.132643	1	6.583609	–0.620182	3.205563
6	–2.082937	0.999935	3.028316	1	4.984778	–1.162613	3.692773
1	–1.392220	1.565161	2.397334	1	5.250602	–1.383506	1.241350
1	–1.923624	1.328235	4.062794	1	5.668333	0.319720	1.110232
1	–3.094703	1.281886	2.736483	6	3.808802	0.563302	–1.430878
6	–2.607458	–1.241046	4.028908	1	3.119375	0.493959	–2.284002
1	–2.229245	–0.912853	5.004782	6	4.028894	2.057562	–1.156683
1	–2.472205	–2.324746	3.968659	1	4.721923	2.173562	–0.315156
1	–3.678807	–1.036433	4.015255	1	3.088580	2.535618	–0.863707
6	–1.759390	–2.754449	–2.324833	6	4.624931	2.752847	–2.381272
1	–1.734971	–3.847946	–2.273475	1	3.898654	2.719142	–3.203074
1	–1.486822	–2.463168	–3.345936	1	4.797355	3.810608	–2.160661
1	–1.003632	–2.367105	–1.639324	6	5.926621	2.081293	–2.819826
6	–4.090986	0.985348	–3.277250	1	6.318795	2.562768	–3.720604
1	–3.944394	1.554855	–4.201215	1	6.684666	2.219331	–2.037536
1	–5.046281	0.459388	–3.345069	6	5.724908	0.585992	–3.065269
1	–4.175976	1.696366	–2.453021	1	5.055435	0.445766	–3.923699

1	6.674529	0.111568	–3.330623
6	5.122725	–0.114049	–1.843682
1	5.840862	–0.079689	–1.017881
1	4.961340	–1.170401	–2.073073
6	–1.431761	0.461547	–0.057304
7	–2.396983	1.256028	–0.323263
6	–2.497455	2.687992	–0.594269
1	–2.654870	2.809985	–1.671883
6	–1.237668	3.453391	–0.210669
1	–1.014350	3.270495	0.847341
1	–0.381693	3.076804	–0.778830
6	–1.421160	4.952367	–0.455060
1	–1.529345	5.132959	–1.532536
1	–0.521493	5.489895	–0.139787
6	–2.651528	5.497860	0.271400
1	–2.778478	6.563539	0.056818
1	–2.498357	5.411137	1.354751
6	–3.909491	4.721514	–0.120765
1	–4.122834	4.890393	–1.184495
1	–4.777226	5.092029	0.432868
6	–3.730981	3.225484	0.128984
1	–4.613371	2.664492	–0.194534
1	–3.612915	3.036755	1.202253

4–3NATS6

SCF energy = –2683.03578937

79	0.542002	0.095602	–0.388437
17	–2.551436	0.946064	2.576668
15	2.768829	–0.272358	0.293410
5	–2.520275	–0.845186	–0.385669
5	–3.667024	0.722350	1.129587
7	–2.378968	–1.985893	–1.311694
7	–3.599820	–0.635887	0.533111
7	–2.119380	1.503123	–0.674022
6	–1.499249	0.386387	–0.524339
6	–2.959923	–1.903719	–2.654538
1	–2.140718	–1.937657	–3.385982
6	–3.679987	–0.582417	–2.912369
1	–4.519032	–0.433980	–2.232878
1	–4.072702	–0.575951	–3.931879
1	–3.013457	0.274526	–2.802455
6	–3.891826	–3.077952	–2.977245
1	–3.411303	–4.046740	–2.816311
1	–4.207232	–3.037627	–4.022208
1	–4.792264	–3.048790	–2.354821
6	–1.514960	–3.134242	–1.057495
1	–2.143864	–4.037077	–0.934311
6	–0.704016	–2.992607	0.234465
1	–0.377636	–3.979062	0.585342
1	–1.258350	–2.519196	1.046995
1	0.192946	–2.386107	0.071425
6	–0.549270	–3.440585	–2.208861
1	0.169562	–4.206418	–1.901551
1	0.001914	–2.533543	–2.481562
1	–1.054473	–3.811553	–3.101050
6	–4.632876	–1.645627	0.950762
6	–5.941552	–1.478456	0.173883
1	–5.767220	–1.550438	–0.898757
1	–6.430349	–0.527497	0.374041
1	–6.642818	–2.269065	0.453198
6	–4.891624	–1.510732	2.463162
1	–5.648069	–2.235711	2.770811
1	–5.255849	–0.525063	2.751777
1	–3.977814	–1.701186	3.025166
6	–4.173341	–3.091611	0.746255
1	–4.057031	–3.347429	–0.300909
1	–4.930629	–3.755645	1.171119
1	–3.233867	–3.298653	1.263117
6	–1.437216	2.757833	–0.998884
1	–2.238883	3.501681	–1.094582
6	–0.751031	2.689486	–2.364552
1	0.023022	1.913245	–2.340479
6	–0.124205	4.029770	–2.743490
1	0.392502	3.943922	–3.707035
1	–0.912630	4.781160	–2.877958
6	0.842504	4.508050	–1.658228
1	1.284144	5.466713	–1.933159
1	1.664469	3.786291	–1.587215
6	0.144220	4.597985	–0.302480
1	–0.628315	5.376393	–0.348040
1	0.853424	4.916741	0.472518
6	–0.489246	3.263266	0.090632
1	0.305890	2.520160	0.247259
1	–1.480667	2.373645	–3.120263
1	–1.017189	3.344128	1.044030
6	–4.762054	1.893936	0.941648
6	–4.155600	3.273328	1.269467
1	–3.224718	3.453569	0.738583
1	–3.951495	3.375896	2.338195
1	–4.863023	4.061978	0.989777
6	–5.287732	1.960188	–0.505109
1	–5.699500	1.008381	–0.851498
1	–4.484110	2.227792	–1.189695

1	–6.085547	2.707669	–0.582951
6	–5.958863	1.746657	1.911567
1	–5.629521	1.659507	2.948277
1	–6.607899	0.898656	1.683859
1	–6.584443	2.647291	1.848742
6	2.731586	–0.353915	2.144119
1	2.315530	0.639361	2.378945
6	1.710255	–1.358776	2.695341
1	0.740300	–1.226574	2.204200
1	2.030119	–2.386784	2.491178
6	1.553177	–1.182848	4.210497
1	1.115100	–0.195929	4.417007
1	0.835524	–1.921799	4.589395
6	2.896215	–1.313897	4.926373
1	2.765760	–1.164309	6.005957
1	3.279687	–2.334068	4.796509
6	3.912948	–0.316909	4.373820
1	4.883509	–0.449946	4.870732
1	3.585402	0.701156	4.605447
6	4.085925	–0.458552	2.859496
1	4.785066	0.305330	2.502545
1	4.553408	–1.429317	2.640215
6	3.956013	1.110652	–0.040868
1	4.917084	0.802930	0.385631
6	3.514238	2.413840	0.639980
1	2.514753	2.683660	0.281716
1	3.429275	2.280799	1.719771
6	4.487223	3.563898	0.358535
1	4.109518	4.479210	0.820691
1	5.447426	3.347981	0.840283
6	4.713856	3.773019	–1.138964
1	5.459597	4.558272	–1.303450
1	3.786307	4.126721	–1.600221
6	5.152172	2.478229	–1.811154
1	6.141193	2.190295	–1.431822
1	5.265634	2.627243	–2.887904
6	4.164569	1.337823	–1.547630
1	4.547707	0.431623	–2.019097
1	3.201853	1.562395	–2.019454
6	3.121994	–1.964099	–1.888667
1	2.052305	–2.201859	–1.830276
1	3.191549	–1.056068	–2.484875
6	3.635133	–1.737409	–0.452831
1	4.700575	–1.467983	–0.494010
6	3.851482	–3.114385	–2.584016
1	3.431311	–3.255049	–3.586399
1	4.906861	–2.851336	–2.718418
6	3.738490	–4.407790	–1.774036
1	2.688553	–4.722266	–1.742734
1	4.292925	–5.215148	–2.261215
6	4.239030	–4.195145	–0.348247
1	5.318480	–3.976426	–0.368861
1	4.117216	–5.112384	0.239242
6	3.509044	–3.043210	0.346806
1	2.446160	–3.304202	0.455172
1	3.913528	–2.922756	1.351259

4–3NATS7

SCF energy = –2683.05771296

79	–0.785888	–0.134239	–0.321803
17	0.900436	–3.201669	0.403754
15	–2.999818	0.140185	0.287057
5	3.456535	–0.142912	0.056221
5	1.876512	–1.797875	–0.273560
7	4.556376	0.680468	0.569839
7	3.289944	–1.577264	0.077853
7	2.225543	0.467562	–0.457722
6	1.223009	–0.477873	–0.580342
6	5.493615	1.426977	–0.266984
1	5.316967	2.507888	–0.139807
6	5.296688	1.136829	–1.750699
1	5.417692	0.073526	–1.971567
1	6.038788	1.686613	–2.335084
1	4.311250	1.443631	–2.102256
6	6.963075	1.175475	0.099855
1	7.159345	1.325680	1.163716
1	7.607037	1.867128	–0.451651
1	7.265740	0.157666	–0.154616
6	4.635705	0.925024	2.013808
1	5.535021	0.432478	2.424154
6	3.436367	0.354667	2.775139
1	3.614593	0.443240	3.850049
1	3.247815	–0.692666	2.554219
1	2.520622	0.901316	2.542256
6	4.738422	2.418787	2.353867
1	4.711153	2.556860	3.438210
1	3.893854	2.965321	1.921395
1	5.658977	2.880871	1.992238
6	4.283530	–2.619498	0.441088
6	5.719289	–2.114038	0.281826
1	5.945960	–1.306072	0.973288
1	5.901264	–1.756419	–0.734939

1	6.415235	–2.934740	0.478697
6	4.139080	–3.839725	–0.480038
1	4.908795	–4.577119	–0.236015
1	4.270829	–3.559733	–1.527486
1	3.170832	–4.326121	–0.365969
6	4.102779	–3.086086	1.895634
1	4.421429	–2.316627	2.601873
1	4.715823	–3.972381	2.086092
1	3.063491	–3.342404	2.103962
6	2.052330	1.913205	–0.608125
1	3.058554	2.330846	–0.509790
6	1.220549	2.564309	0.504598
1	0.188370	2.198308	0.451907
6	1.233155	4.087069	0.377529
1	0.630274	4.536107	1.174196
1	2.257502	4.454421	0.526542
6	0.734019	4.539565	–0.994439
1	0.799391	5.628680	–1.085384
1	–0.327842	4.281995	–1.098519
6	1.521072	3.862852	–2.116975
1	2.559476	4.219385	–2.095864
1	1.113958	4.149511	–3.091727
6	1.509174	2.340461	–1.972504
1	0.482298	1.972511	–2.081506
1	1.607869	2.262006	1.479074
1	2.094787	1.879195	–2.772797
6	1.557228	–1.636017	–2.417790
6	0.449314	–0.934741	–3.210132
1	0.520775	0.150747	–3.178416
1	–0.545231	–1.220664	–2.858537
1	0.517760	–1.239190	–4.266258
6	2.896330	–1.198143	–2.970056
1	3.735783	–1.732717	–2.525456
1	3.062138	–0.133440	–2.809840
1	2.926824	–1.371094	–4.054327
6	1.342964	–3.133157	–2.650428
1	0.378337	–3.471356	–2.267662
1	2.112878	–3.764961	–2.211411
1	1.348795	–3.318471	–3.734918
6	–4.247889	–0.326889	–1.000013
1	–4.181787	0.513852	–1.702937
6	–3.853515	–1.576699	–1.805010
1	–2.843342	–1.451223	–2.204077
1	–3.818363	–2.458126	–1.158909
6	–4.841607	–1.828570	–2.945083
1	–4.768493	–1.012768	–3.676121
1	–4.564707	–2.745141	–3.474291
6	–6.278631	–1.919887	–2.433242
1	–6.970689	–2.082588	–3.264996
1	–6.373668	–2.791825	–1.772768
6	–6.667596	–0.658628	–1.663078
1	–7.688017	–0.744181	–1.276820
1	–6.662707	0.198890	–2.348415
6	–5.701911	–0.386489	–0.506586
1	–5.979939	0.548599	–0.011091
1	–5.816033	–1.175988	0.242820
6	–3.441394	1.916784	0.604401
1	–4.535769	1.969051	0.670581
6	–2.979395	2.773228	–0.589408
1	–1.895175	2.658274	–0.701682
1	–3.419995	2.415564	–1.524091
6	–3.313486	4.252951	–0.404127
1	–2.930758	4.820577	–1.258114
1	–4.403081	4.386738	–0.402324
6	–2.731476	4.793726	0.899121
1	–3.006156	5.843958	1.035616
1	–1.636745	4.760423	0.845112
6	–3.201937	3.960795	2.088102
1	–4.287600	4.075365	2.205312
1	–2.749717	4.327205	3.014759
6	–2.868231	2.477896	1.912734
1	–3.263165	1.923606	2.767449
1	–1.778715	2.347605	1.918688
6	–2.177958	–0.690904	2.834742
1	–1.280248	–1.117079	2.371991
1	–1.940490	0.350263	3.049638
6	–3.348064	–0.820157	1.836085
1	–4.260524	–0.403820	2.285578
6	–2.469201	–1.438446	4.135637
1	–1.625109	–1.318345	4.821329
1	–3.342049	–0.991650	4.630533
6	–2.730623	–2.918715	3.868422
1	–1.813135	–3.380064	3.483377
1	–2.981025	–3.439745	4.797640
6	–3.848725	–3.092941	2.843804
1	–4.795907	–2.741567	3.274708
1	–3.988251	–4.152212	2.607367
6	–3.570862	–2.317470	1.553792
1	–2.675572	–2.723347	1.066294
1	–4.402690	–2.474153	0.866713

4–5NACy

SCF energy = –2683.09589629

79	–0.800161	–0.033364	–0.255129
17	0.933147	–2.708591	1.096018
15	–3.062030	0.155589	0.223298
5	3.524231	–0.068510	–0.012452
5	1.903325	–1.815224	–0.342482
7	4.634156	0.849255	0.243256
7	3.365216	–1.452385	0.089074
7	2.167814	0.554531	–0.392955
6	1.218890	–0.341983	–0.406399
6	5.438709	1.399926	–0.849456
1	5.329043	2.495998	–0.850463
6	4.944836	0.908159	–2.207378
1	5.026790	–0.178623	–2.287945
1	5.550387	1.349339	–3.002944
1	3.906084	1.180223	–2.397052
6	6.942872	1.101263	–0.741877
1	7.333268	1.249674	0.266849
1	7.498666	1.766199	–1.410122
1	7.166209	0.073930	–1.034333
6	4.983596	1.240071	1.608744
1	5.843453	0.643154	1.962041
6	3.826159	1.006068	2.586584
1	4.205951	0.981462	3.611420
1	3.288577	0.073644	2.415453
1	3.103951	1.821928	2.523399
6	5.377772	2.717855	1.723233
1	5.547116	2.966631	2.774390
1	4.568308	3.356603	1.353411
1	6.287491	2.973737	1.177840
6	4.389775	–2.388924	0.626008
6	5.798324	–2.032396	0.141567
1	6.140411	–1.085836	0.551602
1	5.831668	–1.970099	–0.949907
1	6.503566	–2.807600	0.455390
6	4.127285	–3.830470	0.192117
1	4.863795	–4.486670	0.663741
1	4.238961	–3.942086	–0.886139
1	3.137105	–4.173014	0.488890
6	4.379325	–2.362910	2.163666
1	4.767859	–1.420329	2.551333
1	5.016098	–3.160393	2.558936
1	3.367641	–2.511044	2.545189
6	1.974758	2.006122	–0.557815
1	2.982715	2.426790	–0.501530
6	1.148388	2.665301	0.549171
1	0.125952	2.271335	0.523874
6	1.115183	4.181279	0.358089
1	0.512789	4.642704	1.147603
1	2.129727	4.586031	0.471339
6	0.570092	4.560544	–1.019246
1	0.603884	5.646024	–1.156213
1	–0.486928	4.272793	–1.081445
6	1.341515	3.859212	–2.138286
1	2.367779	4.247999	–2.170852
1	0.892383	4.088394	–3.109442
6	1.382520	2.345814	–1.927924
1	0.369220	1.931087	–1.990902
1	1.553354	2.406223	1.528206
1	1.961307	1.863032	–2.720408
6	1.668960	–2.590716	–1.818664
6	0.345546	–2.146759	–2.478361
1	0.320099	–1.076038	–2.703054
1	–0.514647	–2.381279	–1.841734
1	0.199507	–2.675627	–3.429011
6	2.792398	–2.180865	–2.783269
1	3.778328	–2.493658	–2.431124
1	2.827656	–1.093835	–2.914926
1	2.636463	–2.623703	–3.775515
6	1.568971	–4.126871	–1.778543
1	0.821962	–4.455994	–1.051840
1	2.503789	–4.626002	–1.537642
1	1.259723	–4.502338	–2.762800
6	–4.201409	–0.357138	–1.144199
1	–4.134483	0.492526	–1.835887
6	–3.694385	–1.577473	–1.931408
1	–2.673320	–1.393171	–2.275966
1	–3.643036	–2.459677	–1.287762
6	–4.602692	–1.878429	–3.124328
1	–4.532329	–1.058322	–3.850913
1	–4.246283	–2.777318	–3.635548
6	–6.059611	–2.046504	–2.695031
1	–6.692695	–2.244198	–3.565282
1	–6.146525	–2.923119	–2.039725
6	–6.556490	–0.807614	–1.950835
1	–7.593276	–0.943569	–1.627955
1	–6.552104	0.050312	–2.635807
6	–5.677428	–0.490149	–0.738593
1	–6.030517	0.429993	–0.263002
1	–5.796853	–1.285344	0.004002
6	–3.586512	1.910769	0.528747
1	–4.683433	1.920427	0.564620
6	–3.121263	2.785419	–0.650830

1	–2.033561	2.688074	–0.746940
1	–3.542546	2.427490	–1.594086
6	–3.480267	4.259311	–0.465034
1	–3.086930	4.835853	–1.308218
1	–4.571218	4.378309	–0.487060
6	–2.936301	4.801887	0.853531
1	–3.225242	5.848704	0.986301
1	–1.839643	4.779718	0.829024
6	–3.430559	3.958537	2.024963
1	–4.520868	4.056247	2.108574
1	–3.013070	4.328151	2.966523
6	–3.066307	2.482555	1.855215
1	–3.476635	1.918017	2.695540
1	–1.975039	2.372776	1.896208
6	–2.328180	–0.670122	2.800276
1	–1.386832	–1.041311	2.379425
1	–2.159230	0.377449	3.046199
6	–3.439129	–0.841773	1.741120
1	–4.394071	–0.479829	2.147592
6	–2.642398	–1.458805	4.071104
1	–1.839310	–1.307159	4.798428
1	–3.561310	–1.070299	4.531048
6	–2.806690	–2.945210	3.764279
1	–1.848324	–3.346003	3.413313
1	–3.070595	–3.498669	4.670820
6	–3.865770	–3.156976	2.685656
1	–4.849762	–2.864410	3.076490
1	–3.937202	–4.216887	2.423275
6	–3.566895	–2.343784	1.424031
1	–2.626852	–2.692998	0.978537
1	–4.354302	–2.531077	0.693371

4–5NACyI

SCF energy = –2683.07768621

7	–2.751016	–2.309554	–0.351148
15	2.874739	–0.385856	0.136024
6	–1.603684	–3.208534	–0.523882
1	–2.029546	–4.194730	–0.729755
6	–0.816876	–3.377305	0.776546
1	–0.354095	–2.441842	1.102346
1	–0.019730	–4.117787	0.654606
1	–1.478320	–3.716024	1.576944
6	–3.996753	–2.812361	–0.945041
1	–4.743393	–2.062640	–0.714462
6	–3.936793	–2.892673	–2.474667
1	–4.934591	–3.093940	–2.876158
1	–3.281169	–3.697753	–2.820267
1	–3.584756	–1.949595	–2.898613
79	0.554038	–0.237770	–0.022555
5	–2.721415	–0.967691	0.188283
7	–3.761150	–0.210543	0.811044
6	–4.744464	–0.791546	1.777013
6	–6.010300	–1.426476	1.134064
1	–6.262062	–0.972862	0.177016
1	–6.875317	–1.294107	1.788892
1	–5.901135	–2.499237	0.977700
6	–5.238056	0.228922	2.814370
1	–5.805166	1.046958	2.373351
1	–5.894403	–0.293268	3.517010
1	–4.412861	0.660193	3.376787
6	–4.025767	–1.878153	2.597987
1	–4.718055	–2.331669	3.314127
1	–3.626397	–2.669850	1.966486
1	–3.194107	–1.437295	3.154852
5	–3.570741	1.272373	0.374493
17	–3.511867	2.536621	1.830290
6	–4.641780	1.799596	–0.769018
6	–4.377941	3.210512	–1.316426
1	–3.446580	3.284107	–1.876776
1	–4.355817	3.953253	–0.515336
1	–5.180135	3.498674	–2.007599
6	–4.626886	0.828568	–1.960390
1	–3.619238	0.709950	–2.376569
1	–5.274300	1.188758	–2.769778
1	–4.981278	–0.164978	–1.678601
6	–6.070982	1.867415	–0.203926
1	–6.777007	2.159039	–0.992173
1	–6.141043	2.615522	0.590500
1	–6.420801	0.921894	0.203777
6	–4.484750	–4.151308	–0.376531
1	–5.535028	–4.304435	–0.641087
1	–3.931859	–5.003878	–0.781818
1	–4.405968	–4.187644	0.711125
6	–0.698689	–2.902544	–1.724523
1	0.042623	–3.699713	–1.847919
1	–1.273039	–2.830971	–2.647976
1	–0.160065	–1.961000	–1.603262
6	3.586047	–1.773717	–0.849793
6	3.255515	–1.585322	–2.340924
6	3.788716	–2.743767	–3.184567
6	3.251383	–4.084797	–2.690280

6	3.570759	–4.287988	–1.210668
6	3.057102	–3.129270	–0.353977
1	4.676192	–1.754492	–0.725190
1	3.663170	–0.642586	–2.716250
1	2.166728	–1.522276	–2.460682
1	3.520804	–2.586310	–4.233451
1	4.885762	–2.750709	–3.139565
1	3.667369	–4.904323	–3.283803
1	2.164644	–4.112350	–2.835932
1	3.135559	–5.225183	–0.850505
1	4.657137	–4.380124	–1.082723
1	3.342198	–3.300915	0.687628
1	1.961501	–3.113518	–0.380252
6	2.607827	0.145268	2.896155
6	3.426226	–0.665662	1.876039
6	4.929872	–0.519240	2.136480
1	3.155576	–1.717838	2.036312
6	2.967848	–0.262902	4.325492
1	1.538171	–0.001178	2.722515
1	2.797727	1.215664	2.767498
6	4.467793	–0.132699	4.588926
1	2.399752	0.346556	5.033967
1	2.658301	–1.302859	4.490841
6	5.279930	–0.930543	3.568679
1	4.705301	–0.463046	5.604438
1	4.754261	0.925446	4.529647
1	6.351680	–0.791763	3.740502
1	5.078287	–2.001620	3.697996
1	5.513075	–1.109340	1.422221
1	5.219192	0.527901	1.993476
6	3.625797	1.150407	–0.569918
1	3.075792	1.245656	–1.516946
6	3.282203	2.393913	0.264162
1	3.822324	2.354481	1.217001
1	2.215054	2.410793	0.506828
6	3.679070	3.671642	–0.475897
1	3.067850	3.769797	–1.381109
1	3.452085	4.543559	0.144844
6	5.159308	3.655522	–0.856993
1	5.414420	4.555017	–1.425026
1	5.767635	3.680958	0.056703
6	5.513940	2.403650	–1.660534
1	4.992021	2.430339	–2.625748
1	6.584787	2.385913	–1.885015
6	5.121903	1.125003	–0.913746
1	5.718057	1.047137	0.000147
1	5.372203	0.252665	–1.523770
6	–1.501047	0.040577	–0.034834
7	–2.010281	1.235695	–0.113348
6	–1.090419	2.327493	–0.548617
1	–0.122752	2.026347	–0.130008
6	–1.284966	3.753884	–0.036849
1	–2.210430	4.197275	–0.400438
1	–1.347085	3.751163	1.049442
6	–0.092792	4.610041	–0.482885
1	0.819069	4.250396	0.012916
1	–0.241183	5.638243	–0.139601
6	0.119785	4.582240	–1.995395
1	0.997364	5.178776	–2.268270
1	–0.741837	5.047965	–2.490121
6	0.270974	3.148434	–2.500283
1	1.191859	2.711431	–2.088717
1	0.377215	3.130165	–3.589529
6	–0.910466	2.280902	–2.072998
1	–0.744255	1.243027	–2.377476
1	–1.819864	2.614053	–2.579403

4–5NACyM

SCF energy = –2683.12117601

79	–0.654242	0.058337	–0.705744
17	0.198470	–3.066551	–1.849497
15	–2.606297	0.268702	0.527040
5	2.821023	–0.627023	0.068113
5	1.268682	–1.732087	–1.209444
7	3.755553	–0.279976	1.147859
7	2.234746	–1.950501	–0.178845
7	2.297959	0.337636	–0.842490
6	1.221403	–0.246350	–1.683862
6	5.129385	0.098306	0.826751
1	5.213265	1.194315	0.697069
6	5.579304	–0.528793	–0.494893
1	5.679963	–1.614018	–0.406534
1	6.553032	–0.125019	–0.784828
1	4.878749	–0.325589	–1.306749
6	6.118862	–0.297758	1.927665
1	5.934346	0.221136	2.870838
1	7.138291	–0.052620	1.617123
1	6.072202	–1.372468	2.123406
6	3.255654	0.048061	2.480805
1	3.815742	–0.541840	3.223840
6	1.782196	–0.325951	2.627866

1	1.422718	–0.048618	3.622985	1	–0.702837	–0.837262	–3.600142
1	1.602693	–1.390558	2.488977	1	0.658945	–1.835661	–4.109003
1	1.171683	0.204528	1.890401	1	0.221504	–0.410970	–5.044846
6	3.408476	1.527319	2.878145	6	–4.132175	0.502043	–0.494362
1	3.241863	1.642638	3.953624	1	–4.011101	1.534451	–0.847265
1	2.673989	2.152425	2.362398	6	–4.153419	–0.369272	–1.761901
1	4.400008	1.927117	2.656051	1	–3.214898	–0.244012	–2.309399
6	2.617219	–3.265621	0.407505	1	–4.215180	–1.429456	–1.502251
6	3.730267	–3.173827	1.459740	6	–5.342012	–0.003250	–2.651949
1	3.454748	–2.576354	2.326983	1	–5.210466	1.018447	–3.031679
1	4.650351	–2.766337	1.048407	1	–5.360899	–0.659423	–3.527250
1	3.942192	–4.187948	1.811068	6	–6.662981	–0.093516	–1.888036
6	3.161699	–4.167952	–0.713353	1	–7.497167	0.193017	–2.535752
1	3.497062	–5.125262	–0.303176	1	–6.840299	–1.136359	–1.593898
1	4.018780	–3.684849	–1.191546	6	–6.639391	0.786975	–0.639189
1	2.416618	–4.374608	–1.479820	1	–7.578083	0.690192	–0.084946
6	1.416281	–3.930676	1.099816	1	–6.561224	1.839654	–0.940557
1	1.054980	–3.308958	1.922560	6	–5.460303	0.439471	0.274263
1	1.715377	–4.894678	1.521489	1	–5.446254	1.125576	1.126455
1	0.587533	–4.106812	0.418399	1	–5.611851	–0.562946	0.688450
6	2.570880	1.759233	–0.589310	6	–2.630226	1.774639	1.619441
1	3.134320	1.746091	0.342923	1	–3.642831	1.860596	2.034513
6	1.336435	2.614054	–0.275498	6	–2.336540	3.029149	0.774118
1	0.644542	2.642154	–1.120597	1	–1.375852	2.897433	0.265276
6	1.708479	4.043312	0.124981	1	–3.086964	3.151926	–0.011684
1	0.796902	4.639120	0.247191	6	–2.281837	4.302472	1.618991
1	2.205235	4.034155	1.104120	1	–2.031338	5.151611	0.975469
6	2.642715	4.697862	–0.890633	1	–3.274554	4.509511	2.039644
1	2.909313	5.708011	–0.562980	6	–1.269566	4.172496	2.753976
1	2.122019	4.806577	–1.851261	1	–1.251534	5.084724	3.358038
6	3.896383	3.848266	–1.090803	1	–0.263640	4.052403	2.332238
1	4.441231	3.781107	–0.138980	6	–1.600962	2.962230	3.621402
1	4.574742	4.325908	–1.804742	1	–2.572039	3.118737	4.109265
6	3.535602	2.442980	–1.573714	1	–0.863586	2.848853	4.422142
1	3.123821	2.515873	–2.580707	6	–1.648981	1.675721	2.796405
1	0.792675	2.135318	0.546739	1	–1.928929	0.846274	3.449830
1	4.440921	1.834566	–1.653171	1	–0.644377	1.459060	2.414965
6	1.250573	0.086578	–3.211003	6	–1.468448	–1.628071	2.238942
6	0.794324	1.520921	–3.535921	1	–0.796304	–1.910996	1.420986
1	1.342124	2.292366	–3.005176	1	–0.978543	–0.802476	2.751195
1	–0.266064	1.646027	–3.291024	6	–2.823163	–1.208003	1.632084
1	0.913719	1.719951	–4.606520	1	–3.512633	–0.917105	2.436935
6	2.670588	–0.155313	–3.749222	6	–1.616106	–2.813928	3.189522
1	2.966843	–1.195469	–3.578645	1	–0.636424	–3.072563	3.603304
1	3.412524	0.477733	–3.264693	1	–2.248244	–2.529091	4.041440
1	2.717661	0.033143	–4.827352	6	–2.226167	–4.014497	2.472040
6	0.303432	–0.809952	–4.028688	1	–1.525825	–4.364688	1.704279

1	–2.373617	–4.845994	3.168055
6	–3.549472	–3.632900	1.813302
1	–4.290285	–3.403655	2.591014
1	–3.948866	–4.477407	1.243379
6	–3.408448	–2.420962	0.888265
1	–2.746925	–2.673481	0.049522
1	–4.386075	–2.192477	0.462676

4–3N4

SCF energy = –2222.66038890

79	0.633446	0.311185	–0.129872
15	2.953154	0.013218	–0.042250
5	–2.351421	1.788565	–0.181019
5	–3.705140	–0.075025	–0.263839
7	–3.654561	1.344454	–0.560365
7	–2.241535	–0.579006	–0.236436
7	–4.842013	–0.827618	0.140378
6	–1.420599	0.436954	–0.184805
6	–1.737085	3.155124	0.371564
6	–1.007059	2.800330	1.693807
1	–0.588151	3.710396	2.135076
1	–0.178597	2.102520	1.555410
1	–1.689100	2.367438	2.433725
6	–2.705239	4.288102	0.741056
1	–3.434449	3.966789	1.489176
1	–3.248008	4.700808	–0.108885
1	–2.142311	5.117703	1.181351
6	–0.698926	3.697080	–0.631864
1	–0.154033	4.537254	–0.187413
1	–1.168254	4.059761	–1.550370
1	0.042074	2.943741	–0.913786
6	–4.726001	2.101482	–1.284055
6	–5.573937	1.137814	–2.124899
1	–6.174080	0.465511	–1.516802
1	–4.941882	0.531070	–2.780084
1	–6.248283	1.717294	–2.758889
6	–5.645537	2.888139	–0.348568
1	–6.396400	3.423517	–0.935288
1	–5.103297	3.622492	0.240885
1	–6.177978	2.229056	0.335955
6	–4.031389	3.040911	–2.279015
1	–4.774341	3.588331	–2.863030
1	–3.411906	2.467900	–2.974868
1	–3.397790	3.776411	–1.788313
6	–5.506322	–0.294158	1.356763
1	–5.050418	0.688471	1.504836
6	–7.019706	–0.054549	1.276607
1	–7.604668	–0.947479	1.492778
6	–5.144643	–1.129872	2.586707
1	–5.563282	–0.677995	3.489250
1	–4.060592	–1.195541	2.712071
1	–5.539335	–2.146660	2.518397
1	–7.298842	0.695322	2.021849
1	–7.327634	0.321122	0.300624
6	–5.071638	–2.218308	–0.294543
1	–4.504718	–2.913692	0.340637
6	–6.530301	–2.669494	–0.216490
1	–6.886152	–2.795916	0.805005
1	–6.617616	–3.642916	–0.705055
1	–7.193173	–1.975051	–0.736811
6	–4.624455	–2.373274	–1.752663
1	–4.558219	–3.430514	–2.019719
1	–3.651867	–1.925050	–1.967866
1	–5.350636	–1.900890	–2.417798
6	–1.813713	–1.991057	–0.070124
1	–2.720035	–2.586340	–0.111484
6	–1.199271	–2.225479	1.312984
1	–1.924975	–1.941481	2.081464
1	–0.332658	–1.569154	1.441202
6	–0.767049	–3.680216	1.487736
1	–0.274404	–3.800291	2.456660
1	–1.651833	–4.328990	1.509413
6	0.156346	–4.126906	0.355025
1	1.083992	–3.539497	0.391458
1	0.442712	–5.173063	0.491185
6	–0.512780	–3.931022	–1.004683
1	–1.398403	–4.575753	–1.070056
1	0.155345	–4.242903	–1.812271
6	–0.916848	–2.472342	–1.214064
1	–0.010732	–1.860688	–1.263917
1	–1.433843	–2.344007	–2.169746
6	3.468338	–0.271428	1.703889
1	4.562359	–0.340152	1.716659
6	3.039135	0.915105	2.584220
1	3.476227	1.847858	2.217486
1	1.950568	1.036778	2.512970
6	3.424114	0.696333	4.046845
1	3.082810	1.545246	4.645774
1	4.517215	0.669893	4.137653
6	2.835867	–0.607684	4.581730
1	3.139773	–0.765376	5.619938

1	1.740287	–0.535304	4.584410
6	3.263890	–1.794382	3.720734
1	2.805620	–2.718175	4.085613
1	4.348884	–1.932497	3.805812
6	2.896557	–1.590589	2.249832
1	1.803452	–1.583289	2.148197
1	3.259761	–2.440901	1.665950
6	3.989546	1.376176	–0.743347
1	4.132343	1.078476	–1.790724
6	5.380582	1.522447	–0.104709
1	5.925694	0.575344	–0.132983
1	5.275674	1.791652	0.952094
6	6.190740	2.614846	–0.806546
1	7.165248	2.714872	–0.320649
1	6.388140	2.313631	–1.843080
6	5.448621	3.950561	–0.796479
1	5.345107	4.300842	0.238560
1	6.030918	4.710536	–1.324289
6	4.064064	3.813788	–1.427307
1	4.173576	3.575043	–2.492798
1	3.524121	4.763578	–1.376392
6	3.238755	2.718671	–0.751685
1	3.000859	3.017632	0.276706
1	2.281510	2.603876	–1.267407
6	3.373588	–1.522570	–0.965967
1	2.748616	–2.280023	–0.474366
6	4.835707	–1.972010	–0.870861
1	5.475107	–1.237321	–1.374581
1	5.166192	–2.018054	0.171244
6	5.020183	–3.336867	–1.538637
1	6.070683	–3.635291	–1.484720
1	4.452392	–4.089977	–0.977170
6	4.545342	–3.317640	–2.991786
1	4.640007	–4.313059	–3.433947
1	5.196898	–2.656050	–3.576437
6	3.102281	–2.824690	–3.102366
1	2.430002	–3.547979	–2.622305
6	2.922680	–1.460514	–2.433481
1	3.517277	–0.715245	–2.975790
1	1.879026	–1.137961	–2.506306
1	2.799400	–2.764875	–4.151494
7	–2.723562	–1.034945	–1.692375
15	2.429554	–0.416065	0.094821
6	–2.069789	–0.847154	–3.007639
1	–2.854815	–0.949217	–3.758880
6	–1.039828	–1.931665	–3.313403
1	–0.177709	–1.859150	–2.646792
1	–0.684058	–1.837689	–4.343431
1	–1.477737	–2.924782	–3.191577
6	–4.179967	–1.269217	–1.778452
1	–4.515261	–1.463249	–0.761970
6	–4.928350	–0.027867	–2.265799
1	–6.007236	–0.200992	–2.245203
1	–4.661031	0.240165	–3.292029
1	–4.714441	0.834719	–1.627981
79	0.054096	–0.678361	–0.169397
5	–2.013396	–0.986054	–0.474676
7	–2.882156	–1.085110	0.799534
6	–2.942082	–2.437267	1.447629
6	–4.383991	–2.856753	1.741264
1	–4.890665	–2.188698	2.431618
1	–4.389241	–3.852574	2.190589
1	–4.972221	–2.907904	0.821554
6	–2.089729	–2.399803	2.720577
1	–2.464558	–1.677195	3.443923
1	–2.075707	–3.382714	3.198259
1	–1.061314	–2.127025	2.470497
6	–2.347484	–3.502120	0.513085
1	–2.413471	–4.476808	1.001070
1	–2.892275	–3.567524	–0.429478
1	–1.295198	–3.315755	0.289130
5	–3.386335	0.118298	1.251844
6	–4.437230	0.691383	2.328880
6	–4.288119	2.221946	2.487212
1	–4.483618	2.764503	1.557408
1	–3.293580	2.506007	2.847640
1	–5.011909	2.589904	3.219649
6	–5.846214	0.432951	1.746770
1	–5.966481	0.888565	0.757607
1	–6.607222	0.873408	2.399735
1	–6.070891	–0.629528	1.644739
6	–4.332412	0.111916	3.749025
1	–5.083353	0.584123	4.390594
1	–3.354441	0.315676	4.194492
1	–4.504774	–0.961181	3.804133
6	–4.542930	–2.502470	–2.607899
1	–5.606634	–2.723447	–2.489185

4–3NP1

SCF energy = –2222.62005625

1	–4.362345	–2.364030	–3.676703
1	–3.980491	–3.380550	–2.284385
6	–1.500485	0.559164	–3.183536
1	–1.125035	0.694130	–4.201562
1	–2.275609	1.310576	–3.006322
1	–0.674662	0.738260	–2.492283
6	3.263700	–0.789912	–1.510804
6	2.738053	0.165315	–2.597773
6	3.365834	–0.124955	–3.960726
6	3.136626	–1.577863	–4.370930
6	3.675091	–2.532403	–3.307496
6	3.063831	–2.254617	–1.932442
1	4.338543	–0.618166	–1.381420
1	2.920379	1.209171	–2.322480
1	1.649610	0.047481	–2.676396
1	2.951279	0.557207	–4.708944
1	4.443465	0.077183	–3.917064
1	3.609694	–1.779807	–5.335828
1	2.061064	–1.751598	–4.505453
1	3.479906	–3.571070	–3.588727
1	4.765419	–2.426452	–3.244457
1	3.512813	–2.930150	–1.199113
1	1.991064	–2.484799	–1.956367
6	2.321484	–1.676736	2.623909
6	3.123606	–1.616605	1.312856
6	4.627717	–1.513130	1.591125
1	2.941456	–2.573301	0.804489
6	2.802231	–2.837468	3.496966
1	1.254603	–1.784850	2.406508
1	2.433378	–0.740987	3.180268
6	4.304750	–2.752778	3.767074
1	2.246357	–2.845186	4.439122
1	2.575877	–3.785800	2.993174
6	5.100130	–2.678520	2.463559
1	4.631218	–3.610745	4.361198
1	4.515077	–1.859298	4.369080
1	6.168292	–2.572628	2.673007
1	4.981869	–3.618036	1.909110
1	5.197597	–1.486363	0.656945
1	4.835378	–0.574045	2.116518
6	2.945442	1.320596	0.485272
1	2.323902	1.899927	–0.209199
6	2.532024	1.737272	1.903896
1	3.130190	1.180600	2.633202
1	1.485071	1.472199	2.090164
6	2.762640	3.232468	2.133183
1	2.100538	3.812739	1.477007
1	2.491784	3.494602	3.160125
6	4.214334	3.617159	1.849570
1	4.355098	4.693481	1.981898
1	4.866721	3.126880	2.582962
6	4.633316	3.195781	0.442511
1	4.058417	3.769670	–0.296519
1	5.685225	3.438909	0.269087
6	4.406858	1.700185	0.205259
1	5.075898	1.127219	0.853575
1	4.683791	1.454695	–0.822898
6	–2.770569	1.318438	0.363161
7	–2.297490	2.242907	–0.125419
6	–1.594715	3.354270	–0.698542
1	–1.867366	3.364626	–1.758918
6	–0.088333	3.111898	–0.556540
1	0.140370	2.967157	0.505175
1	0.180971	2.186014	–1.068794
6	0.688381	4.304706	–1.110070
1	0.530918	4.374269	–2.193072
1	1.758395	4.132740	–0.965449
6	0.260119	5.610533	–0.441106
1	0.804403	6.452548	–0.875237
1	0.527011	5.579790	0.622786
6	–1.246276	5.833693	–0.580869
1	–1.498667	5.979738	–1.638074
1	–1.549045	6.746403	–0.062803
6	–2.044669	4.653805	–0.023836
1	–3.117002	4.800844	–0.175561
1	–1.876702	4.562386	1.055033

4–3NP2

SCF energy = –2222.62014658

7	2.857067	–0.271858	1.794025
15	–2.233716	–0.430343	0.115335
6	2.248818	0.336516	2.988547
1	3.064664	0.507135	3.693276
6	1.273573	–0.639080	3.648620
1	0.476821	–0.912533	2.950498
1	0.813505	–0.194580	4.535736
1	1.777329	–1.559006	3.951126
6	4.268055	–0.694267	1.941849
1	4.533997	–1.174977	1.000630
6	5.181158	0.524920	2.084323

1	6.229175	0.216281	2.059012	1	–4.137392	0.206728	1.430660
1	5.023302	1.057174	3.026273	1	–3.332454	2.341167	0.472250
1	5.013690	1.228693	1.264879	1	–1.824293	2.201944	1.366794
79	0.061283	–0.049656	0.119600	1	–3.357265	3.762822	2.492298
5	2.251392	–0.406444	0.530364	1	–4.624490	2.550005	2.546418
7	2.634006	–1.372831	–0.524678	1	–3.504160	2.674894	4.749747
6	2.617147	–2.845881	–0.527006	1	–1.937527	2.400464	4.004508
6	4.008201	–3.462986	–0.356460	1	–2.787741	0.280317	4.967254
1	4.706762	–3.092619	–1.105265	1	–4.274745	0.424283	4.045630
1	3.943409	–4.547964	–0.468521	1	–2.691821	–1.149405	2.955347
1	4.420283	–3.262667	0.634070	1	–1.460297	0.102021	2.901578
6	2.004951	–3.279694	–1.863485	6	–2.114541	–3.054014	–0.869839
1	2.632439	–2.985057	–2.706052	6	–2.585336	–2.224498	0.333471
1	1.883375	–4.364850	–1.897422	6	–4.023445	–2.599236	0.720795
1	1.022603	–2.818398	–1.998234	1	–1.934794	–2.485013	1.180589
6	1.709453	–3.325054	0.610992	6	–2.191547	–4.547702	–0.555300
1	1.670538	–4.416295	0.626009	1	–1.096229	–2.775164	–1.159528
1	2.069980	–2.984009	1.583070	1	–2.757922	–2.839799	–1.730015
1	0.687501	–2.953858	0.481847	6	–3.608381	–4.947901	–0.142732
5	2.990294	–0.319747	–1.375389	1	–1.870887	–5.124325	–1.427459
6	3.966497	–0.016284	–2.579215	1	–1.487850	–4.784374	0.252995
6	3.090767	0.350729	–3.795180	6	–4.112911	–4.098369	1.023746
1	2.428038	1.191183	–3.574397	1	–3.641153	–6.008032	0.121815
1	2.476512	–0.494800	–4.123102	1	–4.281752	–4.821581	–0.999840
1	3.725599	0.640143	–4.639367	1	–5.146914	–4.359469	1.264643
6	4.834087	1.202507	–2.196470	1	–3.519741	–4.318486	1.920504
1	4.228766	2.085335	–1.988899	1	–4.358809	–2.032386	1.593345
1	5.515155	1.443439	–3.019481	1	–4.707634	–2.350669	–0.096654
1	5.453037	0.995248	–1.316478	6	–2.934216	0.269654	–1.436820
6	4.909759	–1.163320	–2.958491	1	–2.773927	1.345164	–1.278649
1	5.531378	–0.866155	–3.809751	6	–2.144468	–0.096517	–2.705470
1	4.381132	–2.072432	–3.253568	1	–2.265623	–1.159574	–2.932411
1	5.589477	–1.414390	–2.139505	1	–1.072275	0.069479	–2.557329
6	4.488828	–1.713622	3.055808	6	–2.643194	0.731514	–3.890760
1	5.525829	–2.057873	3.042281	1	–2.424925	1.791541	–3.706112
1	4.303246	–1.291038	4.046739	1	–2.091548	0.452657	–4.792664
1	3.844804	–2.587256	2.933265	6	–4.145740	0.548007	–4.105733
6	1.604243	1.699723	2.748927	1	–4.488928	1.177219	–4.931092
1	1.446568	2.203319	3.705742	1	–4.344032	–0.489595	–4.402542
1	2.240029	2.333735	2.128101	6	–4.935273	0.868831	–2.836404
1	0.626590	1.612298	2.268558	1	–4.835466	1.936597	–2.603489
6	–3.068663	0.440938	1.505583	1	–6.001148	0.682663	–2.992793
6	–2.896173	1.963933	1.400896	6	–4.438119	0.047306	–1.643785
6	–3.536984	2.688040	2.585895	1	–4.624747	–1.015132	–1.837329
6	–3.007078	2.166594	3.919465	1	–5.003891	0.310808	–0.744793
6	–3.202543	0.655883	4.027695	6	2.060258	0.849622	–0.680581
6	–2.541650	–0.070503	2.856075	7	1.921982	2.038014	–1.038395

6	0.957596	2.989595	–0.532722
1	0.461106	2.592898	0.366120
6	–0.114160	3.225110	–1.604582
1	0.378731	3.550000	–2.527431
1	–0.614162	2.277312	–1.832117
6	–1.123564	4.275921	–1.144246
1	–1.679838	3.892353	–0.280343
1	–1.858664	4.453363	–1.935091
6	–0.431505	5.582200	–0.752943
1	–1.166577	6.302372	–0.383166
1	0.024465	6.031431	–1.643431
6	0.650991	5.339836	0.299970
1	0.184514	4.997032	1.233211
1	1.166858	6.273787	0.537020
6	1.663500	4.296856	–0.174792
1	2.419788	4.111471	0.593786
1	2.194871	4.660797	–1.061112

4–3NP3

SCF energy = –2222.60390807

7	–3.556388	–0.916529	–1.477880
15	2.275246	0.074706	–0.392467
6	–2.889607	–0.406347	–2.705173
1	–3.673774	–0.352556	–3.463132
6	–1.819130	–1.377212	–3.187746
1	–1.008543	–1.457837	–2.454249
1	–1.379313	–1.005528	–4.115373
1	–2.222737	–2.372718	–3.376386
6	–5.033549	–0.747802	–1.300973
1	–5.248299	–1.152216	–0.305079
6	–5.430417	0.721377	–1.297323
1	–6.491306	0.809540	–1.053727
1	–5.283297	1.181492	–2.278257
1	–4.856525	1.273154	–0.549820
79	0.100376	0.127988	0.502928
5	–2.914043	–1.470014	–0.444313
7	–2.316239	–2.072034	0.590830
6	–2.095180	–3.566013	0.553162
6	–3.322511	–4.267361	1.137702
1	–3.531426	–3.950638	2.156557
1	–3.167113	–5.348922	1.143790
1	–4.209172	–4.061140	0.530423
6	–0.818392	–3.926974	1.302865
1	–0.929888	–3.821002	2.378225
1	–0.563264	–4.969419	1.101325
1	0.017789	–3.303513	0.976537
6	–1.938597	–4.002775	–0.906636
1	–1.811741	–5.085860	–0.952516
1	–2.823678	–3.761432	–1.503237
1	–1.065148	–3.544615	–1.373759
5	–1.961359	–0.981182	1.610350
6	–1.720481	–1.105162	3.212968
6	–0.259622	–1.386935	3.619299
1	0.393220	–0.556878	3.330692
1	0.155326	–2.294372	3.179587
1	–0.189197	–1.489629	4.708039
6	–2.097541	0.243140	3.862744
1	–1.443869	1.052561	3.533710
1	–2.000532	0.168239	4.950799
1	–3.124293	0.539093	3.633848
6	–2.639667	–2.162754	3.851318
1	–2.616167	–2.058638	4.940600
1	–2.336672	–3.186926	3.633131
1	–3.682791	–2.041279	3.542620
6	–5.798723	–1.582552	–2.320702
1	–6.867035	–1.541286	–2.098544
1	–5.667392	–1.209742	–3.339389
1	–5.486583	–2.629214	–2.291675
6	–2.294838	0.982308	–2.503970
1	–1.925647	1.366977	–3.458021
1	–3.019235	1.689058	–2.106418
1	–1.455766	0.935755	–1.806508
6	2.658822	1.704468	–1.166429
6	2.574110	2.811456	–0.099537
6	2.785109	4.203255	–0.696678
6	1.817704	4.475276	–1.845923
6	1.936742	3.397198	–2.919490
6	1.706635	2.002274	–2.337101
1	3.683719	1.660498	–1.554463
1	3.306869	2.640378	0.694218
1	1.585573	2.771396	0.376540
1	2.668307	4.954765	0.089551
1	3.816215	4.292367	–1.060582
1	2.005545	5.462681	–2.275820
1	0.789186	4.491845	–1.462568
1	1.218683	3.576212	–3.725123
1	2.933678	3.442384	–3.374919
1	1.822856	1.257683	–3.129632
1	0.669879	1.929155	–1.983315
6	1.726341	–2.510989	–1.391210

6	2.404261	–1.176732	–1.737422
6	3.804817	–1.406601	–2.315210
1	1.787933	–0.720543	–2.524311
6	1.656395	–3.413118	–2.624031
1	0.723113	–2.321794	–0.996542
1	2.276538	–3.024059	–0.595757
6	3.040139	–3.632389	–3.238312
1	1.203482	–4.373066	–2.357211
1	0.994568	–2.952252	–3.369912
6	3.732927	–2.305741	–3.551489
1	2.958172	–4.238090	–4.144775
1	3.658634	–4.206204	–2.536824
1	4.739866	–2.485948	–3.937402
1	3.184791	–1.783748	–4.346361
1	4.287230	–0.456978	–2.565724
1	4.432934	–1.890855	–1.559117
6	3.527132	–0.179001	0.934564
1	3.192977	0.543033	1.693098
6	3.409352	–1.573971	1.568442
1	3.746754	–2.329686	0.849520
1	2.364679	–1.801627	1.807484
6	4.275312	–1.665454	2.825320
1	3.884547	–0.973916	3.582242
1	4.201620	–2.669158	3.253396
6	5.732901	–1.321026	2.518063
1	6.329108	–1.351410	3.433976
1	6.150980	–2.084168	1.849067
6	5.855409	0.051503	1.855210
1	5.547636	0.828747	2.566056
1	6.898368	0.259000	1.600639
6	4.988088	0.150645	0.596549
1	5.366072	–0.546854	–0.157098
1	5.076757	1.152719	0.167546
6	–1.948670	0.417443	1.039181
7	–2.608013	1.484095	0.922901
6	–1.952028	2.739450	0.548926
1	–1.195902	2.556596	–0.233164
6	–1.230879	3.326474	1.768779
1	–1.955534	3.422340	2.586116
1	–0.464532	2.620524	2.109094
6	–0.602809	4.684660	1.460316
1	0.205133	4.553809	0.729766
1	–0.139130	5.090827	2.363982
6	–1.628053	5.667973	0.896504
1	–1.141982	6.611800	0.633137
1	–2.368728	5.903185	1.670550
6	–2.342789	5.078009	–0.319361
1	–1.621095	4.947617	–1.137451
1	–3.103001	5.772415	–0.687707
6	–2.982616	3.730746	0.014422
1	–3.482790	3.317160	–0.866476
1	–3.759122	3.861836	0.777321

4–3NTS1

SCF energy = –2222.61163068

7	–2.879038	–0.248948	–1.790802
15	2.352930	–0.422535	–0.139192
6	–2.311488	0.415424	–2.982715
1	–3.156618	0.640777	–3.635640
6	–1.393475	–0.523941	–3.761816
1	–0.507882	–0.784392	–3.174242
1	–1.058277	–0.053069	–4.690055
1	–1.911209	–1.451285	–4.017048
6	–4.347140	–0.412138	–1.813342
1	–4.601425	–0.928108	–0.889353
6	–5.043262	0.949430	–1.763080
1	–6.120934	0.818199	–1.639529
1	–4.887634	1.530843	–2.676001
1	–4.674685	1.538914	–0.919070
79	–0.022657	–0.332174	–0.342530
5	–2.112145	–0.618584	–0.676601
7	–2.728127	–1.409155	0.459590
6	–2.912447	–2.882705	0.383463
6	–4.385514	–3.297637	0.431577
1	–4.896770	–2.905525	1.309102
1	–4.462943	–4.387086	0.464099
1	–4.924591	–2.959293	–0.455817
6	–2.121936	–3.507143	1.540782
1	–2.505739	–3.201677	2.512742
1	–2.170072	–4.597659	1.487704
1	–1.071827	–3.207249	1.477997
6	–2.303334	–3.407679	–0.922972
1	–2.413927	–4.493235	–0.964685
1	–2.790032	–2.988385	–1.803143
1	–1.235603	–3.178607	–0.988513
5	–2.950061	–0.464650	1.448975
6	–3.949117	–0.255137	2.681635
6	–3.570083	0.956202	3.553652
1	–3.601396	1.897727	3.002017
1	–2.569647	0.853307	3.985546

1	–4.275926	1.046480	4.384795
6	–5.330947	0.024045	2.047455
1	–5.307346	0.894389	1.383302
1	–6.066192	0.236238	2.830803
1	–5.699073	–0.824773	1.466508
6	–4.054539	–1.464506	3.625572
1	–4.776609	–1.242994	4.418024
1	–3.099480	–1.682280	4.111986
1	–4.397640	–2.372578	3.131361
6	–4.853923	–1.267075	–2.972914
1	–5.929582	–1.429567	–2.868554
1	–4.693579	–0.792989	–3.944658
1	–4.370372	–2.245572	–2.992981
6	–1.637603	1.754792	–2.687151
1	–1.453689	2.290729	–3.622109
1	–2.273107	2.379679	–2.055059
1	–0.675616	1.620199	–2.187570
6	3.152981	0.733638	–1.333222
6	2.747747	2.179211	–1.000830
6	3.324140	3.181692	–1.999850
6	2.932912	2.827355	–3.432418
6	3.358284	1.400854	–3.773383
6	2.777811	0.389119	–2.783834
1	4.239731	0.637020	–1.221248
1	3.061187	2.448600	0.011656
1	1.651372	2.248948	–1.016857
1	2.982294	4.190212	–1.746183
1	4.417385	3.194120	–1.910612
1	3.380161	3.535613	–4.134943
1	1.844404	2.919487	–3.545866
1	3.044317	1.139353	–4.787747
1	4.453237	1.334116	–3.760036
1	3.126039	–0.613805	–3.045450
1	1.684015	0.378616	–2.880783
6	2.148102	–3.232414	0.093361
6	2.980080	–2.107201	–0.546265
6	4.478187	–2.335474	–0.311752
1	2.794324	–2.164282	–1.627616
6	2.586947	–4.596410	–0.443429
1	1.082853	–3.076007	–0.105110
1	2.268052	–3.217215	1.181571
6	4.084861	–4.828167	–0.242615
1	2.010808	–5.386836	0.046240
1	2.349617	–4.654972	–1.513368
6	4.910144	–3.698148	–0.857888
1	4.378449	–5.788532	–0.674718
1	4.300981	–4.891267	0.831503
1	5.974784	–3.853249	–0.662620
1	4.788405	–3.706561	–1.948408
1	5.074449	–1.539153	–0.767985
1	4.681467	–2.307438	0.764483
6	2.898470	0.139616	1.531186
1	2.333436	1.075664	1.637485
6	2.409160	–0.793818	2.647906
1	2.968948	–1.735023	2.608374
1	1.352804	–1.046484	2.503930
6	2.621426	–0.146131	4.017273
1	1.986542	0.746317	4.094807
1	2.295109	–0.830782	4.805161
6	4.084437	0.246300	4.224854
1	4.208653	0.748917	5.187829
1	4.697882	–0.662530	4.268165
6	4.591269	1.140431	3.092748
1	4.061057	2.101662	3.119519
1	5.651606	1.366825	3.234325
6	4.381015	0.489714	1.722160
1	4.993568	–0.413717	1.655151
1	4.732737	1.164589	0.937130
6	–2.061133	0.834474	1.024816
7	–1.754949	1.961528	1.195670
6	–0.944261	3.047716	0.711339
1	–0.474113	2.686187	–0.213140
6	0.143394	3.375016	1.735840
1	–0.332673	3.620635	2.691359
1	0.759508	2.486147	1.902790
6	0.992478	4.550350	1.250904
1	1.549294	4.252574	0.355021
1	1.737004	4.798722	2.011724
6	0.131335	5.770299	0.921948
1	0.758817	6.578507	0.537616
1	–0.335459	6.147320	1.839852
6	–0.957532	5.418731	–0.092657
1	–0.494311	5.146287	–1.049730
1	–1.591064	6.286333	–0.291697
6	–1.822840	4.259241	0.400932
1	–2.575858	3.988307	–0.344114
1	–2.358222	4.550029	1.311635

4–3NTS2

SCF energy = –2222.59844118

7	–2.897397	–0.662298	–1.825168
15	2.325387	0.063975	–0.216685
6	–2.148606	–0.044754	–2.941476
1	–2.825089	–0.080084	–3.797355
6	–0.916726	–0.873759	–3.286517
1	–0.211966	–0.893373	–2.449291
1	–0.397968	–0.434670	–4.141579
1	–1.183008	–1.901848	–3.538518
6	–4.390675	–0.758786	–1.927290
1	–4.708256	–1.273771	–1.015155
6	–5.038020	0.619386	–1.927555
1	–6.124657	0.512711	–1.898629
1	–4.788959	1.183042	–2.830542
1	–4.728270	1.192329	–1.051995
79	0.035835	0.176168	0.331423
5	–2.417347	–1.127644	–0.650340
7	–2.404283	–2.000321	0.410851
6	–2.322453	–3.485151	0.212453
6	–3.680482	–4.123751	0.499596
1	–4.022847	–3.925307	1.512590
1	–3.618789	–5.206917	0.369739
1	–4.435482	–3.746822	–0.196246
6	–1.211798	–4.034937	1.106769
1	–1.432936	–3.917833	2.164539
1	–1.073820	–5.101235	0.915178
1	–0.266224	–3.526627	0.896935
6	–1.936965	–3.776895	–1.240956
1	–1.827022	–4.854091	–1.377096
1	–2.694586	–3.434393	–1.947335
1	–0.982500	–3.313010	–1.504398
5	–2.388159	–1.098724	1.577585
6	–2.543254	–1.334302	3.141155
6	–1.096771	–1.426799	3.692232
1	–0.521610	–0.523756	3.465555
1	–0.542370	–2.283583	3.300055
1	–1.130983	–1.528295	4.782122
6	–3.201913	–0.095196	3.784512
1	–2.628516	0.816184	3.619083
1	–3.285700	–0.250518	4.865142
1	–4.207325	0.082488	3.394363
6	–3.350547	–2.555434	3.604577
1	–3.411028	–2.560339	4.697509
1	–2.913901	–3.511049	3.314624
1	–4.378245	–2.522179	3.231341
6	–4.823890	–1.613862	–3.113619
1	–5.900138	–1.789461	–3.052826
1	–4.633953	–1.125991	–4.072214
1	–4.326700	–2.585706	–3.117250
6	–1.792777	1.414356	–2.680208
1	–1.367952	1.858471	–3.583825
1	–2.661986	2.001710	–2.386494
1	–1.052690	1.489023	–1.883356
6	2.879898	1.687049	–0.896783
6	2.585538	2.785192	0.143888
6	2.871813	4.188813	–0.388389
6	2.124604	4.449591	–1.693305
6	2.489231	3.398507	–2.738358
6	2.190634	1.984459	–2.238905
1	3.961868	1.639055	–1.067450
1	3.161958	2.612126	1.057390
1	1.527217	2.728824	0.431607
1	2.590125	4.924764	0.370174
1	3.949340	4.309161	–0.554660
1	2.349026	5.451797	–2.067681
1	1.042188	4.419501	–1.506977
1	1.946823	3.575882	–3.671590
1	3.556268	3.482787	–2.978878
1	2.504168	1.259378	–2.995652
1	1.106026	1.870268	–2.121776
6	1.918679	–2.528642	–1.260695
6	2.638523	–1.196270	–1.521641
6	4.098894	–1.438150	–1.918581
1	2.133835	–0.740989	–2.385181
6	1.977831	–3.415841	–2.503778
1	0.880350	–2.344208	–0.968273
1	2.383847	–3.052943	–0.420621
6	3.423353	–3.651344	–2.946582
1	1.481051	–4.370477	–2.304982
1	1.419064	–2.934070	–3.317375
6	4.167804	–2.332149	–3.159971
1	3.445956	–4.248525	–3.862109
1	3.942670	–4.238782	–2.179076
1	5.212509	–2.524827	–3.418503
1	3.728916	–1.798460	–4.012638
1	4.616943	–0.492310	–2.104697
1	4.623570	–1.930637	–1.092370
6	3.328715	–0.225013	1.303351
1	2.889760	0.498385	2.005043
6	3.085294	–1.621811	1.894556
1	3.516232	–2.377797	1.228537
1	2.011153	–1.828294	1.962074

6	3.740322	–1.749542	3.270060
1	3.253542	–1.056440	3.967569
1	3.576943	–2.756030	3.665634
6	5.235891	–1.440408	3.198330
1	5.683313	–1.497225	4.194161
1	5.734125	–2.206447	2.590308
6	5.490122	–0.064112	2.584023
1	5.096033	0.711522	3.252899
1	6.564186	0.120367	2.494348
6	4.830841	0.076901	1.209014
1	5.307987	–0.612855	0.505650
1	5.003226	1.085568	0.824090
6	–1.936793	0.318700	1.015507
7	–2.642199	1.378496	1.138343
6	–2.088113	2.649950	0.705620
1	–1.329020	2.491249	–0.077262
6	–1.371575	3.303040	1.896882
1	–2.088293	3.426833	2.717131
1	–0.588885	2.625174	2.256611
6	–0.779661	4.655653	1.501958
1	0.009696	4.501549	0.753746
1	–0.299316	5.117438	2.369541
6	–1.844448	5.586984	0.921375
1	–1.389503	6.528275	0.600063
1	–2.568557	5.840947	1.705009
6	–2.579062	4.926174	–0.245868
1	–1.877593	4.779584	–1.078934
1	–3.368591	5.584341	–0.618936
6	–3.171055	3.576221	0.160568
1	–3.668265	3.108234	–0.694476
1	–3.937923	3.712630	0.931597

4–3NTS3

SCF energy = –2222.59722672

7	3.644513	0.063222	1.487266
15	–2.506235	0.016333	0.332581
6	2.777088	0.424871	2.633519
1	3.271666	0.035110	3.527416
6	1.415686	–0.254252	2.518786
1	0.857403	0.117947	1.654304
1	0.823702	–0.030143	3.408524
1	1.489133	–1.341136	2.439275
6	5.123486	0.319889	1.499445
1	5.555915	–0.492833	0.903267
6	5.521006	1.620586	0.815043
1	6.609088	1.658271	0.720072
1	5.209896	2.498288	1.384170
1	5.087926	1.682742	–0.183542
79	–0.407143	–0.049534	–0.700825
5	3.197120	–0.654062	0.433105
7	3.016251	–1.777907	–0.327682
6	3.590339	–3.100101	0.135871
6	4.886410	–3.373074	–0.626876
1	4.734889	–3.388163	–1.703042
1	5.298745	–4.340192	–0.329681
1	5.634363	–2.607817	–0.401532
6	2.542695	–4.188973	–0.085109
1	2.333585	–4.356099	–1.137541
1	2.899619	–5.133043	0.331109
1	1.605823	–3.930487	0.416607
6	3.907361	–3.064754	1.634941
1	4.265435	–4.050882	1.935602
1	4.693087	–2.352281	1.885960
1	3.024639	–2.840537	2.237645
5	2.214583	–1.439971	–1.526832
6	1.876471	–2.178687	–2.903224
6	0.531145	–2.931946	–2.774390
1	–0.282677	–2.257974	–2.490535
1	0.556591	–3.742681	–2.043399
1	0.268554	–3.370818	–3.742918
6	1.670452	–1.059967	–3.953511
1	0.860451	–0.379210	–3.680392
1	1.415454	–1.503012	–4.921403
1	2.572806	–0.457324	–4.089544
6	2.934834	–3.129757	–3.483466
1	2.622627	–3.451248	–4.482162
1	3.082529	–4.039002	–2.899957
1	3.904244	–2.636739	–3.600159
6	5.706720	0.200518	2.902231
1	6.794606	0.256314	2.833282
1	5.382008	1.015596	3.553160
1	5.452066	–0.747729	3.380744
6	2.595254	1.930894	2.786219
1	2.041475	2.138799	3.705096
1	3.546110	2.460738	2.849994
1	2.027370	2.340149	1.947981
6	–2.833068	1.745922	0.890591
6	–2.858301	2.675802	–0.336358
6	–3.050601	4.141151	0.054579
6	–1.999880	4.596332	1.064880

6	–2.000358	3.690720	2.293600
6	–1.785746	2.225360	1.910887
1	–3.817709	1.766618	1.372902
1	–3.645873	2.375900	–1.033623
1	–1.909610	2.570319	–0.878240
1	–3.012551	4.763161	–0.844463
1	–4.050686	4.276433	0.484941
1	–2.179060	5.634610	1.356599
1	–1.007250	4.570399	0.597506
1	–1.224140	4.000603	2.999691
1	–2.957549	3.791176	2.820131
1	–1.815818	1.610126	2.814747
1	–0.781470	2.108656	1.481071
6	–1.788735	–2.378962	1.671263
6	–2.467767	–1.012162	1.863862
6	–3.801651	–1.158690	2.604585
1	–1.793425	–0.427884	2.504303
6	–1.592018	–3.070163	3.022217
1	–0.824962	–2.253449	1.166389
1	–2.397908	–3.016702	1.022885
6	–2.912709	–3.208878	3.780164
1	–1.133648	–4.052443	2.872736
1	–0.886646	–2.483192	3.626210
6	–3.599118	–1.853978	3.952652
1	–2.743646	–3.675056	4.754622
1	–3.577111	–3.882206	3.224111
1	–4.563261	–1.976869	4.453517
1	–2.988811	–1.213628	4.602546
1	–4.277104	–0.183938	2.750736
1	–4.488387	–1.758858	1.997550
6	–3.907428	–0.435021	–0.777675
1	–3.662878	0.127155	–1.689891
6	–3.874170	–1.925395	–1.150651
1	–4.110538	–2.528093	–0.266011
1	–2.869535	–2.217421	–1.475452
6	–4.899591	–2.234304	–2.242599
1	–4.616309	–1.710625	–3.164090
1	–4.880892	–3.303396	–2.472556
6	–6.303887	–1.803888	–1.819202
1	–7.018646	–1.997722	–2.623456
1	–6.625860	–2.412253	–0.964111
6	–6.337571	–0.326540	–1.428256
1	–6.124695	0.289167	–2.311444
1	–7.337742	–0.045139	–1.087127
6	–5.314247	–0.007024	–0.334586
1	–5.595639	–0.528576	0.585091
1	–5.344976	1.062648	–0.109953
6	1.584259	–0.033164	–1.276060
7	2.392315	0.971993	–1.229445
6	1.804924	2.305132	–1.035365
1	1.011616	2.242006	–0.269375
6	1.151154	2.768645	–2.344195
1	1.918682	2.786003	–3.127436
1	0.399406	2.036930	–2.657076
6	0.516885	4.150763	–2.192632
1	–0.322614	4.083891	–1.489260
1	0.093080	4.471598	–3.148554
6	1.519708	5.184086	–1.679690
1	1.022902	6.144282	–1.512795
1	2.284038	5.357806	–2.447112
6	2.199115	4.705331	–0.396986
1	1.455893	4.652467	0.411217
1	2.953354	5.428145	–0.073420
6	2.837931	3.329046	–0.583750
1	3.306486	3.003916	0.343647
1	3.633637	3.383814	–1.336488

4–5tOTf

SCF energy = –2464.29399074

79	2.503808	–0.013127	–0.112300
6	0.578339	0.617828	0.251104
7	–1.438306	1.905833	–0.111347
7	–0.397759	–0.144769	0.621285
5	–0.045032	2.090777	–0.027129
5	–1.781253	0.615141	0.670573
15	4.675958	–0.662076	–0.584863
6	5.565240	0.445842	–1.721502
1	6.582744	0.092821	–1.906117
1	5.602206	1.447664	–1.290141
1	5.025697	0.505243	–2.668200
6	4.828943	–2.304897	–1.351910
1	4.273221	–2.320908	–2.290998
1	4.394063	–3.054428	–0.688229
1	5.874488	–2.556220	–1.546209
6	5.762238	–0.755420	0.871945
1	5.355527	–1.476255	1.583348
1	5.797049	0.219948	1.360020
1	6.775181	–1.055775	0.593027
6	–4.001094	–1.756365	–1.867218
6	0.976798	3.349349	–0.067496

6	0.417930	4.777002	0.031958
1	–0.227014	5.059446	–0.798447
1	1.249936	5.491696	0.040397
1	–0.141968	4.931604	0.956219
6	1.851416	3.276731	–1.335745
1	2.343603	2.305005	–1.448593
1	2.639529	4.039232	–1.296839
1	1.269963	3.452931	–2.245321
6	1.897879	3.204208	1.168736
1	2.464877	2.269885	1.175182
1	1.327481	3.245214	2.101899
1	2.625885	4.023915	1.191931
6	–2.411385	2.849180	–0.731092
6	–3.761031	2.184659	–1.034386
1	–4.417154	2.937390	–1.480746
1	–4.263192	1.798116	–0.151203
1	–3.653650	1.374157	–1.750362
6	–2.685523	4.108459	0.136565
1	–2.414906	5.028712	–0.384586
1	–2.128059	4.084516	1.070397
1	–3.744100	4.188031	0.393031
6	–1.852721	3.245932	–2.108718
1	–1.722023	2.352689	–2.724650
1	–0.891525	3.750944	–2.045091
1	–2.548054	3.916597	–2.621823
6	–2.295138	0.836796	2.226914
6	–2.453537	–0.459642	3.045480
1	–3.161139	–1.165754	2.608261
1	–2.832868	–0.215351	4.044637
1	–1.508447	–0.984851	3.194038
6	–1.240539	1.691372	2.955663
1	–0.251631	1.220354	2.952337
1	–1.525994	1.835971	4.003896
1	–1.135340	2.683696	2.508864
6	–3.640131	1.574387	2.335159
1	–4.458412	1.003462	1.892932
1	–3.615915	2.557315	1.867826
1	–3.889190	1.731420	3.391884
6	–0.308226	–1.594735	0.872120
1	–1.295921	–1.893163	1.215634
6	0.688550	–1.981635	1.965351
1	1.710058	–1.735543	1.650666
1	0.497800	–1.405332	2.874836
6	0.595732	–3.483357	2.237977
1	–0.399658	–3.717595	2.634773
1	1.316039	–3.767585	3.011546
6	0.836271	–4.291883	0.961428
1	0.738390	–5.362296	1.167095
1	1.870792	–4.129905	0.625471
6	–0.125763	–3.875845	–0.152455
1	0.092799	–4.427951	–1.071947
1	–1.152563	–4.131599	0.131183
6	–0.050382	–2.373777	–0.419949
1	–0.782208	–2.075941	–1.170855
1	0.940761	–2.117476	–0.816181
16	–3.815003	–1.321448	–0.081219
9	–4.935076	–2.694421	–1.972095
9	–2.861327	–2.234810	–2.362737
9	–4.369009	–0.707243	–2.592824
8	–2.688287	–0.320801	–0.224163
8	–5.050410	–0.721273	0.312141
8	–3.396044	–2.542505	0.542262

4–5tOTfl1

SCF energy = –2464.27930261

79	–1.583677	0.703947	0.818723
6	0.448858	0.798741	0.633621
7	2.835584	0.351225	0.917886
7	1.085244	1.316135	–0.382896
5	1.584089	0.026233	1.549383
5	2.465500	0.688586	–0.448479
15	–3.799488	0.034589	0.709129
6	–4.081860	–1.515066	1.607636
1	–5.100645	–1.878600	1.451932
1	–3.907297	–1.359817	2.673842
1	–3.362191	–2.246979	1.234778
6	–4.212384	–0.351805	–1.014969
1	–3.441818	–1.019136	–1.407101
1	–4.199017	0.565722	–1.606791
1	–5.195757	–0.822236	–1.090769
6	–5.110030	1.162727	1.276914
1	–5.046230	2.104014	0.728404
1	–4.973405	1.373786	2.338892
1	–6.097440	0.720959	1.122233
6	–0.014356	–3.750179	–1.923260
6	1.145761	–0.710754	2.909749
6	2.168974	–1.572228	3.667840
1	2.514776	–2.404913	3.050615
1	1.682689	–2.011267	4.546053
1	3.040146	–1.033466	4.038148
6	–0.030792	–1.677210	2.650387
1	–0.891775	–1.201446	2.181123
1	–0.372826	–2.087156	3.607951

1	0.256783	–2.503283	2.002838
6	0.634844	0.404395	3.855685
1	–0.175968	0.985203	3.405297
1	1.418521	1.107550	4.151923
1	0.237107	–0.046817	4.771901
6	4.198172	0.433064	1.517337
6	5.120591	1.288837	0.640911
1	6.017524	1.548105	1.208137
1	4.635662	2.225339	0.348662
1	5.451632	0.770121	–0.254081
6	4.078998	1.204625	2.840276
1	3.414412	0.725827	3.551694
1	3.698068	2.212789	2.653331
1	5.060054	1.294728	3.313840
6	4.852653	–0.934880	1.726244
1	4.927840	–1.480476	0.786326
1	4.295924	–1.554583	2.421498
1	5.863023	–0.806189	2.125786
6	3.125846	0.318209	–1.867855
6	2.014533	–0.022015	–2.893306
1	2.466608	–0.548189	–3.739546
1	1.535727	0.865767	–3.307556
1	1.243641	–0.668124	–2.480987
6	3.965516	1.449958	–2.500491
1	3.412599	2.392501	–2.570540
1	4.232653	1.162960	–3.523394
1	4.894784	1.657752	–1.971534
6	3.975606	–0.962105	–1.753322
1	3.386829	–1.780959	–1.332637
1	4.871341	–0.836502	–1.147194
1	4.309790	–1.271242	–2.749165
6	0.547949	2.299759	–1.344645
1	1.350878	2.459011	–2.066389
6	0.321207	3.636757	–0.632158
1	–0.466126	3.509683	0.120729
1	1.230316	3.928387	–0.095561
6	–0.077570	4.716962	–1.638985
1	0.770043	4.915689	–2.308121
1	–0.281986	5.655143	–1.114434
6	–1.287369	4.296096	–2.474726
1	–1.515316	5.064234	–3.220049
1	–2.166727	4.221514	–1.821429
6	–1.053338	2.943950	–3.150242
1	–1.943510	2.635386	–3.706055
1	–0.245909	3.035389	–3.889319
6	–0.695982	1.871762	–2.122455
1	–0.556093	0.892069	–2.575805
1	–1.537556	1.761351	–1.430457
16	–0.546640	–2.267419	–0.964996
9	–1.045153	–4.292528	–2.571792
9	0.504834	–4.675431	–1.115198
9	0.916311	–3.417994	–2.823876
8	0.709526	–1.819671	–0.369975
8	–1.083270	–1.376700	–1.977613
8	–1.524433	–2.782528	–0.029402

4–5tOTfIs

SCF energy = –2464.28919247

79	–1.433664	0.977065	0.328049
6	0.546564	0.496562	0.332183
7	2.460384	–1.043942	0.084487
7	1.593664	1.176862	–0.022847
5	1.036570	–1.005208	0.713140
5	2.878927	0.303078	0.062889
15	–3.749514	1.090027	0.360757
6	–4.440076	0.301044	1.849951
1	–5.531994	0.269523	1.806681
1	–4.124753	0.854260	2.735255
1	–4.043798	–0.714654	1.915329
6	–4.503021	0.184063	–1.022845
1	–4.115897	–0.839385	–1.012485
1	–4.220347	0.653260	–1.966147
1	–5.591229	0.165294	–0.933620
6	–4.544321	2.732613	0.310737
1	–4.256926	3.247523	–0.611559
1	–4.198841	3.328934	1.160437
1	–5.631498	2.642234	0.348089
6	–1.388422	–3.168006	–1.794678
6	0.978405	–1.275072	2.342146
6	1.668325	–2.576461	2.756212
1	1.200999	–3.450798	2.297777
1	1.607520	–2.710379	3.844493
1	2.722964	–2.570232	2.486135
6	–0.448147	–1.303100	2.917526
1	–1.031409	–0.413885	2.651162
1	–0.404807	–1.340386	4.013081
1	–1.015568	–2.179213	2.604978
6	1.718653	–0.121508	3.043795
1	1.241345	0.846054	2.878301
1	2.757578	–0.050331	2.708873
1	1.751392	–0.294398	4.126664
6	2.981319	–2.162898	–0.743131
6	2.397603	–1.974881	–2.159797

1	2.672895	–2.809379	–2.813911
1	2.793793	–1.054214	–2.602397
1	1.313459	–1.898949	–2.133762
6	4.502633	–2.171790	–0.882329
1	4.986174	–2.346551	0.078488
1	4.879282	–1.242332	–1.310296
1	4.792851	–2.979028	–1.554713
6	2.608647	–3.552792	–0.208562
1	1.543671	–3.691357	–0.054143
1	3.119319	–3.758184	0.732655
1	2.931618	–4.304931	–0.928859
6	4.302654	1.048558	0.305986
6	4.089413	2.250868	1.259074
1	3.470487	3.047138	0.855526
1	5.060894	2.706847	1.485546
1	3.649709	1.944554	2.213976
6	5.330402	0.158272	1.037770
1	4.863413	–0.479045	1.794093
1	6.067573	0.788074	1.546688
1	5.889648	–0.482958	0.366537
6	4.948556	1.571934	–0.992154
1	4.320482	2.295520	–1.525026
1	5.169391	0.764036	–1.694574
1	5.897572	2.071543	–0.764349
6	1.526438	2.528746	–0.619259
1	2.552159	2.830498	–0.799901
6	0.889835	3.576978	0.286911
1	–0.149376	3.301573	0.497908
1	1.404319	3.598320	1.251812
6	0.919743	4.952347	–0.383602
1	1.961919	5.274650	–0.510217
1	0.442046	5.691305	0.265828
6	0.233727	4.909922	–1.745507
1	0.278182	5.895992	–2.226464
1	–0.830823	4.680478	–1.604809
6	0.861992	3.851568	–2.652725
1	0.338781	3.810070	–3.612494
1	1.898271	4.140418	–2.878298
6	0.846865	2.475218	–1.992521
1	1.357547	1.733807	–2.620145
1	–0.186439	2.125445	–1.874541
16	–1.184610	–2.778181	–0.007086
9	–2.528411	–3.831369	–1.964680
9	–0.385890	–3.913285	–2.241484
9	–1.443918	–2.045871	–2.510644
8	0.065129	–1.950762	–0.136374
8	–2.357365	–2.012788	0.325093
8	–0.963534	–4.021777	0.663921

4–5tOTfTS1

SCF energy = –2464.26396398

79	2.172527	–0.363848	–0.273286
6	0.188005	–0.001166	–0.644535
7	–1.954565	–0.245405	–1.740269
7	–0.425443	1.134035	–0.514076
5	–0.912032	–1.067590	–1.206998
5	–1.953634	0.955618	–0.833845
15	4.374946	–0.855970	0.232124
6	4.840778	–2.591592	–0.045913
1	5.884594	–2.774242	0.220575
1	4.686068	–2.841512	–1.096889
1	4.194752	–3.235450	0.553371
6	4.782279	–0.549157	1.977342
1	4.128956	–1.150332	2.611725
1	4.600632	0.502103	2.207668
1	5.825571	–0.792615	2.192138
6	5.619101	0.098923	–0.690038
1	5.463759	1.163542	–0.506008
1	5.496209	–0.082103	–1.759125
1	6.633662	–0.174881	–0.390597
6	–3.050962	–1.383346	2.874345
6	–0.644459	–2.654448	–1.054097
6	–1.888233	–3.563103	–1.053675
1	–2.611705	–3.227280	–0.308016
1	–1.594891	–4.583654	–0.782450
1	–2.401897	–3.637943	–2.010406
6	0.017104	–2.931019	0.317233
1	0.975162	–2.421238	0.445161
1	0.212774	–4.005908	0.408679
1	–0.611596	–2.628114	1.150138
6	0.364910	–3.126905	–2.124510
1	1.301670	–2.560245	–2.069896
1	–0.008738	–3.041346	–3.146183
1	0.614713	–4.180889	–1.952821
6	–2.903137	–0.611220	–2.826141
6	–3.220966	0.606512	–3.706566
1	–3.800323	0.282714	–4.575002
1	–2.295396	1.058377	–4.073871
1	–3.800425	1.372007	–3.207298
6	–2.217459	–1.580504	–3.801475
1	–1.997978	–2.546519	–3.366100
1	–1.284022	–1.149201	–4.175115
1	–2.870897	–1.758120	–4.658999

6	–4.194167	–1.236975	–2.288421
1	–4.702621	–0.570291	–1.595615
1	–3.988911	–2.163391	–1.754998
1	–4.881890	–1.463739	–3.109288
6	–2.956154	2.230147	–0.700979
6	–2.868127	2.934366	0.678800
1	–3.337076	3.921921	0.597117
1	–1.867951	3.085734	1.078391
1	–3.406123	2.375416	1.440060
6	–2.629526	3.299892	–1.774620
1	–1.709513	3.845737	–1.547449
1	–3.431980	4.045340	–1.805406
1	–2.516017	2.901741	–2.781841
6	–4.453562	1.859614	–0.775392
1	–4.681605	1.064624	–0.062399
1	–4.808548	1.551345	–1.755701
1	–5.050789	2.733321	–0.490907
6	0.247556	2.397666	–0.149356
1	–0.520776	3.162279	–0.175989
6	1.276914	2.809499	–1.205641
1	2.061148	2.048951	–1.287706
1	0.785090	2.862493	–2.182565
6	1.912778	4.150418	–0.841061
1	1.151759	4.940580	–0.880646
1	2.671692	4.414508	–1.583916
6	2.519098	4.109528	0.561873
1	2.971031	5.075019	0.809137
1	3.329646	3.367086	0.581697
6	1.464424	3.728660	1.600487
1	1.905068	3.686416	2.600751
1	0.693979	4.509720	1.635874
6	0.812994	2.386628	1.272068
1	0.020208	2.155102	1.985945
1	1.553072	1.584378	1.371016
16	–1.941414	–0.052647	2.238488
9	–2.778244	–1.638079	4.151688
9	–2.889661	–2.516849	2.181987
9	–4.327023	–1.017763	2.777106
8	–2.460684	0.047328	0.850413
8	–2.227041	1.080676	3.074545
8	–0.605171	–0.590054	2.310658

4–5tOTfTS2

SCF energy = –2464.27409762

79	1.859334	0.185249	–0.552890
6	–0.099740	0.748376	–0.663171
7	–2.540596	0.586951	–0.922747
7	–0.664768	1.695529	0.031389
5	–1.311546	–0.149019	–1.332821
5	–2.141468	1.340769	0.227333
15	3.770054	–1.026940	–0.066276
6	3.762278	–2.628455	–0.920382
1	4.605719	–3.248817	–0.607072
1	3.803099	–2.472557	–1.999847
1	2.822857	–3.127334	–0.675038
6	3.776001	–1.459987	1.696872
1	2.818095	–1.926410	1.931856
1	3.870351	–0.553153	2.296561
1	4.593410	–2.145451	1.933871
6	5.418779	–0.325066	–0.385642
1	5.525919	0.617699	0.153493
1	5.530450	–0.124627	–1.452651
1	6.204383	–1.014155	–0.066052
6	–1.422111	–3.336768	1.939259
6	–0.969039	–1.014061	–2.668861
6	–1.982077	–2.109386	–3.055841
1	–2.037871	–2.859137	–2.262088
1	–1.642631	–2.619898	–3.964501
1	–2.994257	–1.768543	–3.253812
6	0.362171	–1.792048	–2.572335
1	1.230898	–1.131471	–2.511280
1	0.496471	–2.382012	–3.486518
1	0.390436	–2.477452	–1.727142
6	–0.749029	0.000790	–3.815967
1	0.068949	0.687234	–3.567032
1	–1.618217	0.611596	–4.052855
1	–0.456820	–0.525613	–4.732393
6	–3.930041	0.465417	–1.443855
6	–4.819223	1.602899	–0.919220
1	–5.769533	1.594226	–1.457414
1	–4.350034	2.575694	–1.096629
1	–5.057520	1.520332	0.133586
6	–3.945316	0.688560	–2.964987
1	–3.413932	–0.067191	–3.526694
1	–3.507549	1.661596	–3.204289
1	–4.978312	0.687413	–3.322372
6	–4.550073	–0.888039	–1.079505
1	–4.672374	–0.986340	–0.001584
1	–3.922253	–1.715850	–1.402111
1	–5.533377	–0.999648	–1.546821
6	–2.797840	1.603383	1.687178
6	–1.689078	1.523293	2.769960
1	–2.162508	1.425824	3.751773

1	–1.079724	2.425049	2.820505
1	–1.034508	0.660461	2.636423
6	–3.477266	2.978277	1.853569
1	–2.800227	3.805170	1.614245
1	–3.781538	3.108210	2.898413
1	–4.368325	3.102155	1.238599
6	–3.776285	0.476539	2.081571
1	–3.311121	–0.502523	1.959172
1	–4.709672	0.472674	1.524834
1	–4.046425	0.583166	3.137288
6	0.007014	2.903102	0.549308
1	–0.760985	3.442702	1.106305
6	0.410819	3.792750	–0.631720
1	1.173275	3.268633	–1.220374
1	–0.450525	3.943618	–1.290034
6	0.950106	5.134324	–0.133133
1	0.135123	5.692071	0.346464
1	1.280201	5.739872	–0.982448
6	2.092011	4.952042	0.867951
1	2.414979	5.924179	1.252895
1	2.957115	4.515411	0.352383
6	1.684140	4.029754	2.018239
1	2.525826	3.874839	2.699618
1	0.890196	4.505166	2.609536
6	1.196430	2.682447	1.484623
1	0.935646	1.995248	2.289792
1	2.016636	2.214834	0.930745
16	–0.314810	–2.161707	1.046945
9	–0.736202	–3.980526	2.881317
9	–1.930938	–4.232556	1.097249
9	–2.430866	–2.690366	2.525277
8	–1.258027	–1.611439	0.053014
8	0.115185	–1.211223	2.045377
8	0.722578	–3.005355	0.499226

OTf⁻

SCF energy = –961.550996307

8	1.230442	–1.060777	–0.936737
16	0.922708	0.000118	–0.000141
8	1.230380	1.341779	–0.450382
8	1.231763	–0.280817	1.386650
6	–0.930134	–0.000025	0.000235
9	–1.434233	0.245179	–1.222225
9	–1.434410	0.935956	0.823800
9	–1.433934	–1.181492	0.398938

4–5tCl

SCF energy = –1963.02859642

79	–1.763355	–0.428967	0.107333
6	0.292430	–0.212079	0.124630
15	–4.056406	–0.721588	–0.003279
7	2.634368	–0.733588	–0.252967
5	2.485024	0.792919	–0.015876
7	0.900579	0.928464	0.062910
6	0.903813	–2.922287	0.191364
5	1.420041	–1.382906	0.021410
6	0.094975	–2.984854	1.508434
1	–0.739640	–2.280633	1.541553
1	0.732357	–2.772607	2.373405
1	–0.323601	–3.989233	1.648823
6	–0.034177	–3.239906	–0.995666
1	0.523470	–3.331021	–1.932663
1	–0.803942	–2.479168	–1.153681
1	–0.549528	–4.194069	–0.826754
6	4.445889	–2.405319	0.303685
1	5.377334	–2.030170	0.732320
1	4.668633	–3.375974	–0.145336
1	3.759749	–2.560844	1.130267
6	1.875580	–4.112996	0.286008
1	1.293210	–5.042603	0.303203
1	2.463773	–4.099062	1.204543
1	2.568210	–4.190892	–0.550102
6	3.510459	–2.107864	–2.063744
1	3.172087	–1.358380	–2.783227
1	2.711894	–2.838459	–1.947012
1	4.381293	–2.620921	–2.483463
6	5.031907	–0.462358	–1.094177
1	4.805433	0.192101	–1.930935
1	5.891158	–1.081494	–1.369345
1	5.337576	0.153607	–0.250139
6	3.874160	–1.410601	–0.741049
6	3.253215	1.409436	1.350259
6	3.864409	0.279334	2.196940
1	4.690581	–0.223846	1.697468
1	3.123349	–0.484328	2.451904
1	4.259791	0.682618	3.137551
6	4.360809	2.429056	1.034679
1	4.864013	2.736077	1.960536
1	3.953099	3.326863	0.563575
1	5.122807	2.041460	0.356676
6	2.282726	2.129520	2.304766
1	2.816880	2.449198	3.207412

1	1.468646	1.474360	2.628078
1	1.850509	3.031438	1.865652
6	0.227369	2.240002	–0.094412
1	1.036241	2.972517	–0.079411
6	–0.764985	2.607493	1.014420
1	–1.612097	1.911904	1.003629
1	–0.302442	2.515625	1.996254
6	–1.295968	4.025340	0.800506
1	–0.469214	4.742388	0.885033
1	–2.005728	4.277645	1.594842
6	–0.444376	2.355640	–1.470120
1	–1.265524	1.629860	–1.532695
1	0.276172	2.095293	–2.245403
6	–0.992986	3.764665	–1.687195
1	–1.489961	3.822812	–2.660682
1	–0.156914	4.474158	–1.724735
6	–1.954359	4.171872	–0.571055
1	–2.303633	5.198430	–0.720507
1	–2.845004	3.528373	–0.611047
6	–4.939125	0.670456	–0.774891
1	–4.756677	1.578786	–0.197767
1	–6.014605	0.484607	–0.828074
1	–4.548948	0.828221	–1.781915
6	–4.571388	–2.168109	–0.979828
1	–5.659543	–2.259292	–1.020418
1	–4.147439	–3.070344	–0.535607
1	–4.177266	–2.074950	–1.993257
6	–4.895725	–0.946412	1.595478
1	–4.715474	–0.073497	2.225136
1	–4.480758	–1.820316	2.100376
1	–5.971951	–1.081957	1.463595
17	2.901462	1.813150	–1.607600

4–5tLi

SCF energy = –1819.21163870

79	1.784461	–0.316912	–0.372971
3	–0.733632	0.012387	1.579890
8	–2.042853	–1.009520	2.670632
6	–0.223723	–0.165920	–0.375802
15	4.055425	–0.615163	–0.485245
7	–2.539442	–0.549406	–0.947866
5	–2.401225	0.812708	–0.450290
7	–0.999803	1.069921	–0.194321
8	0.233802	0.163818	3.392264
6	–0.874710	–2.846512	–0.587274
5	–1.207031	–1.232882	–0.717991
6	0.007706	–3.362343	–1.741428
1	0.943832	–2.797992	–1.791613
1	–0.472837	–3.267534	–2.717913
1	0.259058	–4.423639	–1.599749
6	–0.061652	–3.075985	0.710708
1	–0.625306	–2.753980	1.591939
1	0.881193	–2.525660	0.706124
1	0.172277	–4.143414	0.835261
6	–2.799469	–1.773598	–3.088953
1	–1.919128	–1.241826	–3.458293
1	–3.477796	–1.943507	–3.930525
1	–2.477632	–2.745924	–2.735577
6	–2.081465	–3.791603	–0.430682
1	–1.735937	–4.804684	–0.185032
1	–2.696477	–3.889647	–1.324845
1	–2.738569	–3.472186	0.384280
6	–4.712068	–1.720821	–1.465008
1	–5.298933	–1.117175	–0.772439
1	–4.391309	–2.618947	–0.938176
1	–5.375940	–2.030359	–2.279315
6	–4.005474	0.296429	–2.779810
1	–4.617427	0.962016	–2.182005
1	–4.614551	–0.016903	–3.632941
1	–3.155752	0.867509	–3.165158
6	–3.508048	–0.939137	–2.007783
6	–3.537583	1.867807	0.109527
6	–4.936770	1.261789	0.339798
1	–4.891256	0.330134	0.906177
1	–5.486280	1.057122	–0.577795
1	–5.553001	1.962788	0.916872
6	–3.086492	2.294868	1.531465
1	–3.836096	2.955021	1.986203
1	–2.137252	2.829518	1.551237
1	–2.981666	1.424219	2.189045
6	–3.734924	3.143018	–0.735814
1	–4.444383	3.821483	–0.243959
1	–4.137631	2.919195	–1.726205
1	–2.810571	3.703395	–0.891560
6	–0.383670	2.392722	–0.262610
1	–1.179162	3.125699	–0.128330
6	0.215275	2.668556	–1.646372
1	0.967990	1.906071	–1.869874
1	–0.576098	2.548188	–2.393849
6	0.839466	4.060328	–1.735143
1	0.055763	4.825785	–1.650377
1	1.303500	4.201825	–2.716903
6	0.627149	2.666829	0.856491

1	1.433265	1.928672	0.798832
1	0.136535	2.531070	1.829262
6	1.230745	4.065994	0.749719
1	1.970877	4.219262	1.543161
1	0.448410	4.821344	0.904802
6	1.866714	4.278959	–0.624203
1	2.302739	5.281075	–0.694264
1	2.691205	3.563774	–0.751975
6	5.075451	0.436266	0.607337
1	4.861776	1.486291	0.397502
1	6.143999	0.251961	0.466670
1	4.811147	0.239420	1.648256
6	4.627553	–2.299107	–0.074415
1	5.710394	–2.400284	–0.185324
1	4.127930	–3.014252	–0.730500
1	4.344433	–2.534137	0.953250
6	4.816650	–0.325507	–2.119689
1	4.622346	0.703905	–2.426844
1	4.348147	–0.986350	–2.851131
1	5.895698	–0.502960	–2.105969
6	1.644861	0.267704	3.410398
1	1.911294	1.135612	2.812355
1	2.101981	–0.623017	2.965329
1	2.004009	0.401678	4.437607
6	–0.242461	–0.912934	4.175516
1	0.042219	–0.776314	5.226969
1	0.192524	–1.852434	3.809409
6	–1.745937	–0.957267	4.046109
1	–2.127704	–1.849577	4.557938
1	–2.208937	–0.069262	4.496800
6	–3.350273	–1.445446	2.354019
1	–3.495890	–2.478498	2.688813
1	–3.438244	–1.387429	1.269913
1	–4.098353	–0.797483	2.825108

4–5tN

SCF energy = –1502.76773553

79	–1.620900	–0.307934	–0.025411
6	0.356093	–0.211326	–0.245911
15	–3.875919	–0.545452	0.200496
7	2.662021	–0.876126	0.069621
5	2.573152	0.580785	–0.102699
7	1.200753	0.961580	–0.145203
6	0.854166	–2.901603	–0.752319
5	1.272073	–1.391723	–0.229936
6	–0.045482	–3.685847	0.221520
1	–0.956595	–3.120837	0.440483
1	0.442820	–3.884175	1.180063
1	–0.341274	–4.657585	–0.207071
6	0.038684	–2.723851	–2.055211
1	0.611065	–2.172176	–2.807203
1	–0.876866	–2.156336	–1.884395
1	–0.232544	–3.704956	–2.481252
6	2.807272	–2.510470	1.930406
1	1.940623	–2.018206	2.377903
1	3.456118	–2.881140	2.732838
1	2.448353	–3.373792	1.379231
6	2.033488	–3.802236	–1.161620
1	1.667268	–4.684226	–1.707952
1	2.611971	–4.182790	–0.317290
1	2.723426	–3.267170	–1.821619
6	4.753552	–2.265036	0.381745
1	5.399996	–1.585758	–0.172885
1	4.393174	–3.018122	–0.317487
1	5.367029	–2.771066	1.138071
6	4.142213	–0.489569	2.039832
1	4.795560	0.243819	1.576543
1	4.727081	–0.997463	2.815365
1	3.322105	0.046374	2.526394
6	3.578709	–1.518002	1.038938
6	3.777196	1.621043	–0.542682
6	5.083970	0.909165	–0.936953
1	4.888186	0.089269	–1.632989
1	5.629538	0.497527	–0.087672
1	5.764947	1.616448	–1.431719
6	3.325082	2.309797	–1.853658
1	4.146341	2.911566	–2.270401
1	2.475105	2.978314	–1.723581
1	3.039437	1.568397	–2.605938
6	4.127951	2.715857	0.481253
1	4.887905	3.401240	0.076019
1	4.530521	2.296346	1.407560
1	3.261515	3.321873	0.759464
6	0.658788	2.301568	–0.040826
1	1.502889	2.995743	–0.045463
6	–0.041522	2.530806	1.307051
1	–0.850883	1.801511	1.418423
1	0.678215	2.316791	2.104718
6	–0.596830	3.948122	1.437655
1	0.232079	4.671002	1.463054
1	–1.132318	4.059836	2.388390
6	–0.239792	2.704715	–1.218767
1	–1.072787	2.000543	–1.289645

1	0.324513	2.595820	–2.150272
6	–0.778041	4.126283	–1.065259
1	–1.444108	4.371203	–1.901556
1	0.050586	4.848989	–1.107054
6	–1.513848	4.295115	0.264603
1	–1.902277	5.316203	0.366783
1	–2.381542	3.620969	0.277729
6	–4.904660	0.854675	–0.383928
1	–4.607736	1.758097	0.153310
1	–5.974033	0.677204	–0.230642
1	–4.707706	1.018595	–1.444707
6	–4.617406	–1.960731	–0.695102
1	–5.696580	–2.038185	–0.528695
1	–4.131438	–2.880274	–0.362593
1	–4.416986	–1.846440	–1.761705
6	–4.567900	–0.795543	1.882560
1	–4.287936	0.055801	2.506526
1	–4.112586	–1.687220	2.317799
1	–5.657928	–0.904093	1.877447

4–5tP

SCF energy = –1209.95061753

79	1.655117	–0.384120	–0.053230
6	–0.373032	–0.097635	–0.116674
7	–2.661047	–0.609205	0.511588
7	–1.032719	1.025490	–0.095760
5	–1.511606	–1.265790	–0.034160
5	–2.533152	0.707913	–0.082538
15	3.937374	–0.812891	0.090402
6	4.334170	–2.565543	0.349865
1	5.414074	–2.714034	0.419182
1	3.943025	–3.155450	–0.480669
1	3.864567	–2.916331	1.270239
6	4.754899	0.058841	1.458186
1	4.294980	–0.229820	2.404586
1	4.630693	1.135525	1.330519
1	5.820741	–0.177889	1.489838
6	4.878202	–0.336488	–1.388355
1	4.753400	0.731614	–1.573637
1	4.502342	–0.881183	–2.255799
1	5.940147	–0.556238	–1.257976
6	–1.262071	–2.693451	–0.692409
6	–2.519411	–3.506998	–1.031357
1	–3.064568	–3.852913	–0.153732
1	–2.240539	–4.401461	–1.597484
1	–3.209857	–2.933056	–1.655805
6	–0.323298	–3.539744	0.190386
1	0.618339	–3.023761	0.407777
1	–0.070138	–4.472563	–0.324942
1	–0.782403	–3.806501	1.145497
6	–0.553597	–2.426428	–2.044017
1	0.419382	–1.941388	–1.927563
1	–1.160648	–1.801492	–2.707658
1	–0.380575	–3.374108	–2.563717
6	–3.741647	–1.144706	1.391110
6	–4.107289	–0.029133	2.379972
1	–4.862314	–0.382530	3.085708
1	–4.511989	0.853116	1.885929
1	–3.227129	0.272395	2.954810
6	–4.985187	–1.635497	0.648308
1	–4.741266	–2.404757	–0.082229
1	–5.504010	–0.830041	0.130844
1	–5.690567	–2.066405	1.362836
6	–3.147939	–2.287643	2.223311
1	–2.240065	–1.959422	2.737220
1	–2.907927	–3.163711	1.624586
1	–3.866117	–2.601860	2.983294
6	–3.579622	1.496200	–0.998494
6	–3.011662	2.740301	–1.706214
1	–2.895450	3.592933	–1.032809
1	–3.709033	3.058377	–2.486591
1	–2.055266	2.549006	–2.196762
6	–3.874422	0.454701	–2.115318
1	–2.963444	0.164781	–2.651700
1	–4.554541	0.892143	–2.852463
1	–4.336271	–0.454055	–1.729398
6	–4.905565	1.929688	–0.352131
1	–4.747995	2.651161	0.454708
1	–5.489161	1.101682	0.045229
1	–5.528055	2.422205	–1.105512
6	–0.443367	2.371982	0.077009
1	–1.282848	3.065590	0.036663
6	0.541729	2.757589	–1.025742
1	1.378101	2.048794	–1.031800
1	0.061169	2.682135	–2.004379
6	1.082589	4.167839	–0.790913
1	0.266320	4.894936	–0.883864
1	1.806108	4.417168	–1.571336
6	1.720137	4.292120	0.592573
1	2.083344	5.310386	0.752900
1	2.598766	3.634804	0.645974
6	0.732347	3.904014	1.692460
1	1.208441	3.960470	2.674852

1	–0.094145	4.625141	1.709158
6	0.177808	2.496346	1.473164
1	–0.571415	2.250132	2.232428
1	0.986431	1.762609	1.576579

BNC

SCF energy = –592.793250190

6	0.435623	2.475382	–0.021381
5	–0.866297	1.602236	0.401198
5	0.690013	0.182897	–0.258956
7	1.236713	1.556621	–0.532273
7	–0.766141	0.304711	–0.190641
6	–1.856635	–0.672701	–0.400513
6	–1.536501	–1.509502	–1.645249
1	–1.477927	–0.860081	–2.523064
1	–0.594411	–2.045887	–1.563026
1	–2.323776	–2.247310	–1.822846
6	–3.152816	0.090937	–0.717001
1	–3.554989	0.611396	0.151146
1	–2.985587	0.823351	–1.511159
1	–3.916291	–0.611637	–1.061066
6	–2.106875	–1.552915	0.828987
1	–1.264077	–2.204218	1.058321
1	–2.298007	–0.932622	1.708076
1	–2.982008	–2.189118	0.669237
6	1.628522	–0.987724	0.328470
6	1.344964	–2.435028	–0.099851
1	1.512412	–2.583306	–1.171024
1	2.030062	–3.108842	0.426679
1	0.335974	–2.770186	0.132957
6	1.397312	–0.869163	1.857032
1	0.366892	–1.093922	2.138245
1	2.053449	–1.567745	2.388543
1	1.628624	0.136662	2.223512
6	3.130677	–0.756584	0.085436
1	3.390848	–0.781137	–0.976375
1	3.479666	0.189345	0.500974
1	3.706628	–1.549232	0.575443
6	2.476080	1.951774	–1.197908
1	3.305652	2.037057	–0.494613
1	2.742958	1.234737	–1.977028
1	2.298778	2.930545	–1.641570
6	–1.957365	2.181857	1.368744
1	–1.478616	2.853324	2.088526
1	–2.642451	2.819468	0.794035
1	–2.564310	1.456362	1.914660

BNCAuPMe3

SCF energy = –1189.13790698

6	0.357062	0.086952	–0.158992
5	1.346859	–1.113229	0.297225
5	2.600124	0.669984	–0.266347
7	1.134929	1.036657	–0.601425
7	2.640629	–0.779020	–0.198020
6	3.778921	–1.737626	–0.338754
6	4.686843	–1.258393	–1.478881
1	4.126037	–1.231797	–2.419567
1	5.110901	–0.271448	–1.304149
1	5.519439	–1.956943	–1.604421
6	3.220105	–3.101752	–0.781463
1	2.678285	–3.618185	0.012458
1	2.557060	–2.988079	–1.646064
1	4.050143	–3.749003	–1.079477
6	4.537254	–1.912704	0.980870
1	5.008984	–0.987931	1.317629
1	3.860108	–2.252461	1.770975
1	5.323011	–2.665554	0.863931
6	3.562256	1.777871	0.367951
6	5.082168	1.648505	0.168604
1	5.366974	1.815137	–0.875628
1	5.584852	2.417762	0.766425
1	5.485882	0.687545	0.486952
6	3.247059	1.577532	1.882843
1	3.564879	0.595308	2.245351
1	3.780837	2.340154	2.462038
1	2.177765	1.694771	2.102020
6	3.210307	3.238411	0.019645
1	3.360612	3.459994	–1.042485
1	2.188091	3.508129	0.295502
1	3.871060	3.907490	0.581961
6	0.622929	2.234941	–1.270089
1	0.278537	2.971858	–0.541333
1	1.399970	2.676300	–1.892783
1	–0.216697	1.937297	–1.901223
6	0.827415	–2.303289	1.171546
1	0.099978	–1.930394	1.904406
1	0.272739	–3.006443	0.532826
1	1.590889	–2.871101	1.706550
79	–1.675790	0.052112	–0.076437
15	–4.011447	–0.098882	0.090458
6	–4.572945	–1.339155	1.310001
1	–4.183981	–1.085737	2.299952

1	–5.666155	–1.372574	1.350595
1	–4.193061	–2.326238	1.032553
6	–4.829365	1.455752	0.594566
1	–4.433916	1.785831	1.558991
1	–4.629178	2.234370	–0.146529
1	–5.910575	1.310005	0.680139
6	–4.835433	–0.573311	–1.470530
1	–4.634270	0.179199	–2.237822
1	–4.444762	–1.533747	–1.817519
1	–5.916557	–0.656784	–1.322795

CAAC

SCF energy = –407.852804841

6	–0.597049	1.286284	0.111439
6	–0.449191	–1.099684	–0.447119
6	0.947990	–0.564475	–0.100464
7	0.649750	0.896060	0.069440
6	1.752051	1.833981	0.216372
1	2.404271	1.544349	1.044471
1	2.348480	1.878415	–0.698399
1	1.322274	2.811569	0.416450
1	–0.515131	–1.288885	–1.522958
6	–1.435971	0.025761	–0.047685
6	1.952768	–0.788256	–1.229329
1	2.950864	–0.422871	–0.972028
1	2.039648	–1.857544	–1.439307
1	1.626076	–0.288136	–2.145029
6	1.491970	–1.143953	1.208885
1	1.651406	–2.220078	1.101208
1	2.451224	–0.696943	1.483141
1	0.793110	–0.984123	2.032201
6	–2.507152	0.249482	–1.116846
1	–3.105738	–0.656770	–1.260821
1	–3.175107	1.064378	–0.828690
1	–2.055816	0.512960	–2.078063
6	–2.114702	–0.245653	1.302914
1	–2.727554	0.607878	1.601508
1	–2.759389	–1.128241	1.235477
1	–1.385324	–0.421956	2.098307
1	–0.655827	–2.047339	0.057448

CAAC2

SCF energy = –1109.40794892

6	0.288696	–0.106907	1.957952
6	–1.245835	–0.095519	2.031512
6	–0.541637	0.142821	–0.318050
1	–1.592168	0.660163	2.740773
1	–1.618487	–1.054270	2.397540
6	–1.752937	0.207199	0.595146
6	–2.264522	1.669802	0.547222
6	–2.891894	–0.747616	0.148073
6	–2.876610	2.102509	–0.782506
1	–1.447732	2.348732	0.822571
1	–3.026116	1.778663	1.332983
6	–3.518051	–0.297618	–1.178539
1	–3.667391	–0.643217	0.922894
6	–4.012206	1.144650	–1.138857
1	–2.104550	2.016676	–1.555501
1	–4.344215	–0.968256	–1.439619
1	–2.773764	–0.385583	–1.974599
1	–4.446891	1.417569	–2.106889
1	–4.815883	1.247104	–0.395028
6	–2.483747	–2.244241	0.124282
1	–1.717532	–2.396327	0.893996
6	–1.870528	–2.700980	–1.201370
1	–1.104638	–2.005941	–1.550341
1	–1.411012	–3.687672	–1.086846
1	–2.628607	–2.782623	–1.985831
6	–3.667866	–3.137963	0.497006
1	–3.387315	–4.195483	0.477223
1	–4.044130	–2.909929	1.498913
1	–4.496770	–3.008520	–0.206894
6	–3.348950	3.550865	–0.719340
1	–2.523450	4.231090	–0.486877
1	–3.782957	3.868463	–1.672073
1	–4.115104	3.681837	0.053496
6	1.843526	0.055097	–0.067341
6	2.500326	–1.132262	–0.415625
6	2.454367	1.307982	–0.237122
6	3.833940	–1.049605	–0.815127
6	3.785313	1.339753	–0.644810
6	4.482420	0.169973	–0.902749
1	4.366055	–1.955791	–1.086289
1	4.280615	2.295185	–0.780603
1	5.522477	0.213072	–1.209549
6	1.774641	–2.461860	–0.529399
1	0.783041	–2.350859	–0.090221
6	1.567646	–2.784220	–2.015125
1	0.973726	–3.694707	–2.134850
1	1.047814	–1.966521	–2.519121
1	2.526483	–2.936283	–2.520220
6	2.483349	–3.614066	0.185387

1	3.448688	–3.844307	–0.274500
1	2.662343	–3.393077	1.239998
1	1.876069	–4.522350	0.130393
6	1.667733	2.603012	–0.129115
1	0.759165	2.402849	0.434547
6	1.215959	3.034990	–1.529890
1	0.624342	2.243123	–1.995112
1	0.601346	3.939256	–1.474532
1	2.075842	3.248180	–2.172879
6	2.416167	3.722351	0.594537
1	2.773958	3.398197	1.575570
1	3.278783	4.078691	0.024358
1	1.754531	4.580548	0.742678
7	0.500384	0.007734	0.459378
6	0.916417	1.072779	2.703247
1	1.988376	1.150852	2.505887
1	0.444331	2.020876	2.440815
1	0.784436	0.927711	3.778483
6	0.888163	–1.402988	2.497734
1	1.971523	–1.432759	2.358482
1	0.687463	–1.475286	3.569868
1	0.451330	–2.280849	2.018470

CAACAuPMe3

SCF energy = –1004.35840875

6	–1.302155	0.102248	–0.039376
6	–2.030989	1.429959	–0.063030
6	–3.494989	1.031174	–0.341703
1	–4.201213	1.615865	0.249530
1	–3.730578	1.205799	–1.394388
7	–2.155254	–0.871325	–0.027132
6	–1.814374	–2.288196	0.011560
1	–2.074623	–2.755399	–0.938483
1	–0.748042	–2.401448	0.189878
1	–2.365912	–2.778753	0.813242
6	–1.850403	2.101937	1.309016
1	–0.796812	2.311794	1.510424
1	–2.389955	3.051886	1.322863
1	–2.231502	1.485620	2.126028
6	–1.473642	2.342982	–1.159742
1	–2.072883	3.255048	–1.219266
1	–0.440865	2.635911	–0.953005
1	–1.500574	1.857864	–2.138984
6	–3.605554	–0.469814	–0.030941
6	–4.211564	–0.748318	1.345675
1	–5.238270	–0.377746	1.366007
1	–4.250735	–1.816498	1.570480
1	–3.656831	–0.248090	2.141476
6	–4.360335	–1.229381	–1.117698
1	–4.470175	–2.291196	–0.885806
1	–5.364693	–0.811131	–1.210356
1	–3.866247	–1.128736	–2.087450
79	0.749057	–0.050787	–0.004792
15	3.074859	–0.135585	0.014095
6	3.842592	1.052405	–1.123907
1	4.931635	0.978123	–1.079910
1	3.511567	0.852916	–2.144293
1	3.542559	2.067005	–0.856583
6	3.758965	–1.747921	–0.463238
1	4.850936	–1.720846	–0.453461
1	3.415026	–2.513988	0.233604
1	3.416943	–2.011962	–1.465198
6	3.814788	0.221920	1.632669
1	3.460302	–0.501330	2.368609
1	4.904563	0.170369	1.575209
1	3.520758	1.220219	1.961210

CBA

SCF energy = –1457.83491131

6	0.955006	0.169991	–0.416706
6	–0.954972	0.169848	0.416657
6	–0.000047	1.069997	–0.000024
7	–0.616717	–1.172525	0.313396
7	0.616933	–1.172440	–0.313506
6	–1.537871	–2.220058	0.019882
6	–1.488390	–2.888485	–1.198874
6	–2.498781	–2.547727	0.969416
6	–2.417082	–3.884856	–1.467023
1	–0.733304	–2.623175	–1.929187
6	–3.434073	–3.531747	0.681977
1	–2.519639	–2.018937	1.913880
6	–3.395595	–4.204615	–0.533768
1	–2.378852	–4.406285	–2.417322
1	–4.190861	–3.779648	1.418199
1	–4.123865	–4.978059	–0.751703
6	1.538234	–2.219830	–0.019926
6	1.488810	–2.888210	1.198857
6	2.499216	–2.547409	–0.969419
6	2.417635	–3.884437	1.467080
1	0.733664	–2.622975	1.929134

6	3.434639	–3.531284	–0.681906
1	2.520026	–2.018658	–1.913906
6	3.396221	–4.204100	0.533869
1	2.379450	–4.405827	2.417402
1	4.191483	–3.779114	–1.418094
1	4.124595	–4.977430	0.751863
8	–2.188176	0.371973	0.888232
8	2.188174	0.372316	–0.888285
6	–2.820980	1.566106	0.527811
6	–3.599625	1.542336	–0.624053
6	–2.694777	2.675443	1.353662
6	–4.299279	2.701948	–0.946235
6	–3.413642	3.813872	0.996266
6	–4.209788	3.828989	–0.140754
1	–4.916250	2.719055	–1.839708
1	–3.337291	4.702287	1.615841
1	–4.760891	4.726356	–0.402364
6	2.820767	1.566546	–0.527824
6	2.694142	2.675940	–1.353527
6	3.599602	1.542850	0.623915
6	3.412774	3.814514	–0.996128
6	4.299018	2.702605	0.946104
6	4.209109	3.829711	0.140758
1	3.336083	4.702980	–1.615588
1	4.916133	2.719772	1.839476
1	4.760025	4.727190	0.402376
6	–3.647278	0.308485	–1.482571
1	–2.666705	0.105030	–1.925517
1	–3.924806	–0.576700	–0.904875
1	–4.364103	0.426654	–2.296999
6	–1.785473	2.640101	2.547479
1	–2.016081	1.794368	3.200875
1	–0.749781	2.529461	2.213052
1	–1.869329	3.558642	3.131024
6	3.647727	0.308918	1.482290
1	2.667282	0.105158	1.925381
1	3.925391	–0.576133	0.904453
1	4.364659	0.427188	2.296609
6	1.784600	2.640501	–2.547160
1	1.868100	3.559129	–3.130617
1	2.015292	1.794901	–3.200699
1	0.749001	2.529553	–2.212542

CCDP

SCF energy = –2052.78273434

6	0.896289	–0.235977	–1.482942
6	–0.021946	–0.173568	1.172478
7	1.242064	–0.123934	1.286913
15	–0.545927	–0.114050	–0.678522
15	2.035185	–0.059394	–0.313974
7	3.034908	1.290968	–0.176543
7	3.359331	–1.082477	–0.215912
6	4.359655	0.935325	0.120844
6	4.541480	–0.388567	0.098718
1	5.110218	1.695082	0.276184
1	5.469542	–0.922237	0.231930
6	3.230412	–2.533945	–0.197305
1	2.204268	–2.733396	–0.520641
6	4.166313	–3.181484	–1.213153
1	3.994104	–4.260252	–1.260225
1	3.998333	–2.757128	–2.204736
1	5.216711	–3.026489	–0.947346
6	3.410872	–3.092711	1.213409
1	2.717133	–2.610028	1.905330
1	3.231611	–4.171698	1.230372
1	4.427756	–2.916010	1.577686
6	2.482334	2.629108	–0.028338
1	1.408144	2.515440	–0.205849
6	3.028337	3.574790	–1.093189
1	2.846407	3.165477	–2.088961
1	2.549862	4.555828	–1.022374
1	4.106936	3.719466	–0.975949
6	2.663561	3.166540	1.390082
1	2.143797	4.121312	1.510984
1	2.266597	2.454171	2.116510
1	3.720943	3.331570	1.618445
6	–0.888976	–0.192436	2.374307
6	–0.398726	0.330940	3.574532
6	–2.178642	–0.723389	2.346121
6	–1.189629	0.340689	4.712264
1	0.608362	0.731395	3.593390
6	–2.965879	–0.726637	3.490731
1	–2.560429	–1.140775	1.423081
6	–2.476695	–0.188338	4.673686
1	–0.801811	0.761047	5.634243
1	–3.963564	–1.151866	3.455693
1	–3.094174	–0.182244	5.566022
7	–1.713211	–1.335808	–0.876126
7	–1.366130	1.342367	–0.923150
6	–2.512640	1.682975	–0.064634
1	–2.801583	0.741253	0.402942
6	–0.849427	2.246167	–1.972021
1	0.175943	1.909598	–2.140423

6	–2.164281	2.643460	1.081920
1	–2.897662	2.539535	1.886954
1	–1.182055	2.418274	1.499924
1	–2.167165	3.686972	0.761643
6	–3.756529	2.170138	–0.810736
1	–3.605287	3.142671	–1.282506
1	–4.079516	1.465458	–1.578124
1	–4.576510	2.281744	–0.095619
6	–1.569393	2.073694	–3.311790
1	–1.111129	2.717024	–4.068860
1	–1.474410	1.042160	–3.660350
1	–2.630460	2.327471	–3.256570
6	–0.772907	3.714782	–1.557015
1	–1.752404	4.192627	–1.481521
1	–0.261000	3.840408	–0.601354
1	–0.203789	4.263273	–2.312376
6	–1.214406	–2.675678	–0.493509
1	–0.570728	–2.490415	0.375991
6	–2.788805	–1.153276	–1.865251
1	–2.730077	–0.099534	–2.132802
6	–2.611612	–1.926509	–3.171949
1	–3.335016	–1.564092	–3.908364
1	–1.608703	–1.783107	–3.578620
1	–2.786153	–2.997920	–3.047146
6	–4.188470	–1.362428	–1.277497
1	–4.300498	–0.831348	–0.329218
1	–4.940100	–0.969958	–1.969633
1	–4.423644	–2.413822	–1.108287
6	–0.334997	–3.380378	–1.539174
1	0.246750	–4.167577	–1.047836
1	–0.927965	–3.859972	–2.319682
1	0.356206	–2.675729	–2.003002
6	–2.312895	–3.621598	–0.010544
1	–1.849740	–4.503705	0.439207
1	–2.960086	–3.163339	0.739123
1	–2.935948	–3.972889	–0.836373

CP

SCF energy = –697.795469925

6	–0.677252	0.610328	–0.000059
6	0.677252	0.610328	–0.000060
6	–0.000000	1.839764	–0.000028
7	1.872217	0.011274	–0.000060
7	–1.872217	0.011273	–0.000058
6	3.078963	0.854866	0.000016
1	3.926745	0.164067	0.000038
6	3.158024	1.703069	1.267568
1	4.090363	2.274605	1.285945
1	2.322905	2.405050	1.310507
1	3.125920	1.070872	2.159036
6	3.158128	1.703122	–1.267492
1	4.090463	2.274671	–1.285766
1	3.126110	1.070962	–2.158990
1	2.323004	2.405094	–1.310476
6	2.000553	–1.444995	–0.000059
1	0.976719	–1.824061	–0.000199
6	2.681606	–1.955415	1.269658
1	2.690676	–3.048653	1.287873
1	3.720013	–1.617921	1.335806
1	2.153799	–1.599923	2.157504
6	2.681928	–1.955396	–1.269611
1	2.690919	–3.048634	–1.287873
1	2.154391	–1.599825	–2.157584
1	3.720380	–1.617983	–1.335456
6	–2.000553	–1.444995	–0.000065
1	–0.976717	–1.824061	–0.000212
6	–2.681600	–1.955421	1.269653
1	–3.720007	–1.617929	1.335807
1	–2.690670	–3.048660	1.287861
1	–2.153789	–1.599935	2.157498
6	–2.681934	–1.955389	–1.269616
1	–2.154401	–1.599813	–2.157590
1	–2.690923	–3.048627	–1.287885
1	–3.720386	–1.617976	–1.335455
6	–3.078963	0.854866	0.000021
1	–3.926746	0.164067	0.000044
6	–3.158132	1.703125	–1.267485
1	–3.126116	1.070967	–2.158983
1	–4.090465	2.274674	–1.285754
1	–2.323007	2.405096	–1.310468
6	–3.158022	1.703065	1.267576
1	–4.090361	2.274602	1.285957
1	–3.125915	1.070867	2.159042
1	–2.322902	2.405047	1.310515

CVP

SCF energy = –998.034368509

6	0.207586	–0.051015	–1.415749
6	0.170544	0.073173	1.359963
1	0.374022	0.091358	2.422579
15	1.306924	0.009820	–0.040551
7	2.337917	–1.299846	–0.017963

7	2.345600	1.325951	0.076232
6	3.342860	1.457751	–0.982772
1	4.143498	2.115647	–0.633051
6	1.751581	2.604328	0.449025
1	1.048520	2.470350	1.271084
6	1.946992	–2.509889	–0.727691
1	1.400854	–2.240458	–1.631517
6	3.146809	–1.523692	1.168081
1	4.058300	–2.062048	0.891901
6	–0.976047	–0.010087	–0.757585
6	–2.374838	–0.013882	–1.323058
6	–2.417938	–0.010572	1.304614
6	–1.025754	0.020434	0.757173
6	–3.106296	–1.264894	–0.799049
1	–4.133135	–1.269939	–1.179398
1	–2.618790	–2.160032	–1.192981
6	–3.101084	–1.280371	0.754455
1	–4.120924	–1.325497	1.149188
1	–2.580273	–2.164276	1.132978
1	–2.429019	–0.008581	2.398162
1	–2.334643	–0.016027	–2.413724
6	–3.157591	1.225919	0.750040
1	–4.190549	1.200051	1.111398
1	–2.705956	2.134312	1.158100
6	–3.112582	1.234778	–0.803058
1	–4.126201	1.258438	–1.216088
1	–2.602505	2.130441	–1.166720
1	3.772119	0.482712	–1.210872
1	2.913537	1.876143	–1.901416
1	2.544456	3.280748	0.779491
1	1.220945	3.074509	–0.389642
1	2.847865	–3.065003	–1.005864
1	1.313543	–3.161733	–0.110615
1	3.438130	–0.568314	1.606387
1	2.612273	–2.114733	1.924649

N1CB

SCF energy = –353.430955843

7	1.021154	–0.835665	0.006560
6	0.061585	–1.723894	0.045817
6	0.621054	0.598517	–0.000921
6	–0.711005	0.724015	0.055181
5	–1.252664	–0.741817	0.016905
6	–2.723542	–1.234698	–0.078775
1	–2.957765	–1.758416	0.860301
1	–3.480820	–0.461682	–0.231237
1	–2.828203	–2.005988	–0.850729
6	–1.495339	2.000209	0.059611
1	–2.044969	2.115088	0.999544
1	–0.881932	2.896089	–0.070957
1	–2.244457	1.997765	–0.738208
6	1.687871	1.636617	–0.084837
1	2.252998	1.546781	–1.017784
1	1.259866	2.638166	–0.046301
1	2.404954	1.545906	0.736206
6	2.437308	–1.184399	0.025951
1	2.955084	–0.781153	–0.848300
1	2.922015	–0.802533	0.928917
1	2.490874	–2.269494	0.015930

N3B3

SCF energy = –386.734415596

7	–1.081576	–0.742294	–0.102183
6	–0.176178	–1.645167	0.109703
7	–0.680326	0.638643	–0.299719
7	0.714103	0.551931	–0.123647
5	1.142272	–0.768179	0.110562
6	2.634508	–1.234940	0.246855
1	2.927904	–1.810140	–0.639325
1	3.369649	–0.435843	0.380059
1	2.734065	–1.926148	1.089734
6	1.443386	1.756860	–0.438862
1	1.106589	2.167298	–1.394526
1	1.331059	2.524394	0.334115
1	2.500583	1.509091	–0.516158
6	–1.293050	1.508647	0.706485
1	–1.070861	1.164879	1.725492
1	–0.917000	2.523014	0.572362
1	–2.370390	1.537953	0.547175
6	–2.510527	–0.962460	–0.286757
1	–3.070548	–0.671686	0.605416
1	–2.867004	–0.390941	–1.145498
1	–2.639661	–2.026583	–0.457363

NBNCAuPMe3

SCF energy = –1502.76773553

79	–1.620900	–0.307934	–0.025411
6	0.356093	–0.211326	–0.245911
15	–3.875919	–0.545452	0.200496
7	2.662021	–0.876126	0.069621

5	2.573152	0.580785	–0.102699
7	1.200753	0.961580	–0.145203
6	0.854166	–2.901603	–0.752319
5	1.272073	–1.391723	–0.229936
6	–0.045482	–3.685847	0.221520
1	–0.956595	–3.120837	0.440483
1	0.442820	–3.884175	1.180063
1	–0.341274	–4.657585	–0.207071
6	0.038684	–2.723851	–2.055211
1	0.611065	–2.172176	–2.807203
1	–0.876866	–2.156336	–1.884395
1	–0.232544	–3.704956	–2.481252
6	2.807272	–2.510470	1.930406
1	1.940623	–2.018206	2.377903
1	3.456118	–2.881140	2.732838
1	2.448353	–3.373792	1.379231
6	2.033488	–3.802236	–1.161620
1	1.667268	–4.684226	–1.707952
1	2.611971	–4.182790	–0.317290
1	2.723426	–3.267170	–1.821619
6	4.753552	–2.265036	0.381745
1	5.399996	–1.585758	–0.172885
1	4.393174	–3.018122	–0.317487
1	5.367029	–2.771065	1.138071
6	4.142213	–0.489569	2.039832
1	4.795560	0.243819	1.576543
1	4.727081	–0.997463	2.815365
1	3.322105	0.046374	2.526394
6	3.578709	–1.518002	1.038938
6	3.777195	1.621043	–0.542682
6	5.083969	0.909165	–0.936953
1	4.888186	0.089269	–1.632989
1	5.629537	0.497527	–0.087672
1	5.764946	1.616448	–1.431719
6	3.325081	2.309797	–1.853658
1	4.146340	2.911566	–2.270401
1	2.475105	2.978314	–1.723581
1	3.039437	1.568397	–2.605938
6	4.127950	2.715857	0.481253
1	4.887904	3.401240	0.076019
1	4.530520	2.296346	1.407560
1	3.261514	3.321873	0.759464
6	0.658788	2.301568	–0.040826
1	1.502889	2.995743	–0.045463
6	–0.041522	2.530806	1.307051
1	–0.850883	1.801511	1.418423
1	0.678215	2.316791	2.104718
6	–0.596830	3.948122	1.437655
1	0.232079	4.671002	1.463054
1	–1.132318	4.059836	2.388390
6	–0.239792	2.704715	–1.218767
1	–1.072787	2.000543	–1.289645
1	0.324513	2.595820	–2.150272
6	–0.778041	4.126283	–1.065259
1	–1.444108	4.371203	–1.901556
1	0.050586	4.848989	–1.107054
6	–1.513848	4.295115	0.264603
1	–1.902277	5.316202	0.366783
1	–2.381542	3.620968	0.277729
6	–4.904660	0.854675	–0.383928
1	–4.607736	1.758096	0.153310
1	–5.974033	0.677203	–0.230642
1	–4.707706	1.018595	–1.444707
6	–4.617406	–1.960731	–0.695102
1	–5.696580	–2.038185	–0.528695
1	–4.131438	–2.880274	–0.362593
1	–4.416986	–1.846440	–1.761705
6	–4.567900	–0.795543	1.882560
1	–4.287936	0.055801	2.506526
1	–4.112586	–1.687220	2.317799
1	–5.657928	–0.904093	1.877447

NHC

SCF energy = –304.758189944

6	0.000000	–0.000000	0.979619
6	0.000000	0.674668	–1.208949
6	–0.000000	–0.674668	–1.208949
7	0.000000	–1.057603	0.121671
7	0.000000	1.057603	0.121671
6	0.000000	2.433785	0.568045
1	0.890372	2.957846	0.211371
1	–0.890372	2.957846	0.211371
1	0.000000	2.425197	1.655758
6	–0.000000	–2.433785	0.568045
1	–0.890372	–2.957846	0.211371
1	0.890372	–2.957846	0.211371
1	–0.000000	–2.425197	1.655758
1	0.000000	–1.381502	–2.023628
1	0.000000	1.381502	–2.023628

NHC2

SCF energy = –924.057751711

6	0.000004	–0.000119	–0.300900
7	–1.055870	–0.000960	0.561900
6	0.673613	0.001436	1.897548
7	1.055870	0.001355	0.561905
6	–0.673622	–0.000065	1.897544
6	–2.422873	–0.002304	0.141321
6	–3.068240	–1.221766	–0.055065
6	–3.073849	1.217691	–0.044561
6	–4.408413	–1.199481	–0.432427
6	–4.412317	1.193282	–0.421490
6	–5.095834	–0.004327	–0.617137
1	–4.926032	–2.142476	–0.588763
1	–4.934795	2.135100	–0.570080
1	–1.389876	–0.000604	2.703111
1	1.389863	0.002536	2.703118
6	2.422875	0.002394	0.141330
6	3.073662	–1.217731	–0.044296
6	3.068432	1.221724	–0.055306
6	4.412136	–1.193602	–0.421234
6	4.408600	1.199160	–0.432656
1	4.934472	–2.135529	–0.569615
1	4.926366	2.142044	–0.589181
6	5.095837	0.003857	–0.617125
6	2.321430	2.516951	0.109380
1	2.978415	3.372868	–0.054625
1	1.495683	2.572176	–0.604892
1	1.884273	2.608384	1.107590
6	2.330368	–2.513509	0.132343
1	1.502177	–2.575889	–0.578519
1	2.988912	–3.368941	–0.027833
1	1.896908	–2.598929	1.132706
6	6.538624	–0.002363	–1.050117
1	7.104489	–0.786841	–0.541392
1	6.622028	–0.185288	–2.126092
1	7.024909	0.952862	–0.840956
6	–2.330747	2.513616	0.131818
1	–1.502194	2.575722	–0.578643
1	–2.989280	3.368914	–0.029122
1	–1.897818	2.599574	1.132368
6	–2.321045	–2.516845	0.109896
1	–1.883619	–2.607853	1.108026
1	–2.977969	–3.372902	–0.053626
1	–1.495474	–2.572225	–0.604567
6	–6.538634	0.001618	–1.050090
1	–7.104845	0.785387	–0.540651
1	–6.622158	0.185456	–2.125898
1	–7.024483	–0.954008	–0.841752

NHCAuPMe3

SCF energy = –901.254452702

6	–1.837446	–0.001030	0.017690
7	–2.652133	1.074874	0.013499
6	–3.972554	0.684268	–0.017290
7	–2.661512	–1.069113	–0.001307
6	–2.252081	–2.466564	–0.010513
1	–2.503858	–2.922709	–0.967953
1	–1.176677	–2.524525	0.142663
1	–2.754328	–2.999974	0.796038
6	–2.219239	2.465256	–0.016570
1	–2.908292	3.068191	0.572840
1	–1.225715	2.542904	0.420253
1	–2.196347	2.832450	–1.042973
6	–3.978711	–0.666185	–0.024872
79	0.220842	–0.000673	0.013834
15	2.539119	–0.000815	–0.008542
6	3.255051	1.295379	–1.058717
1	4.345924	1.243675	–1.041427
1	2.906992	1.171462	–2.085294
1	2.938235	2.276922	–0.702756
6	3.256071	–1.549008	–0.628522
1	4.346856	–1.492624	–0.628172
1	2.941687	–2.381014	0.003534
1	2.907903	–1.735832	–1.645497
6	3.295486	0.244055	1.622822
1	2.974181	–0.547667	2.301277
1	4.385002	0.230518	1.546400
1	2.977668	1.201516	2.038387
1	–4.782222	1.394746	–0.024838
1	–4.794228	–1.369958	–0.036757

NNB3

SCF energy = –292.134930347

7	–1.023681	–0.429949	–0.278439
5	0.000445	0.600862	–0.269128
7	1.030272	–0.422001	–0.275529
6	0.005221	–1.228510	0.215649
6	2.411756	–0.527325	0.120670
1	2.564957	–1.496405	0.599100
1	3.066647	–0.456891	–0.751105

1	2.695928	0.257141	0.829488
6	–0.013092	2.116213	0.086932
1	0.916327	2.623085	–0.183774
1	–0.847050	2.641766	–0.386337
1	–0.142314	2.232191	1.170152
6	–2.403848	–0.542666	0.120958
1	–2.688006	0.233465	0.839072
1	–3.061558	–0.464190	–0.747963
1	–2.553521	–1.517096	0.589534

NNBB

SCF energy = –356.930673079

7	–1.118488	0.655107	0.008835
6	0.000015	1.463731	0.000006
5	–0.866339	–0.760379	0.010479
5	0.866334	–0.760381	–0.010589
7	1.118491	0.655115	–0.008944
6	2.422982	1.300310	–0.023198
1	3.044823	0.936345	0.798670
1	2.946707	1.105886	–0.963419
1	2.281339	2.374637	0.085369
6	1.998986	–1.838046	0.021806
1	2.213410	–2.065864	1.076917
1	1.704972	–2.787091	–0.433929
1	2.945939	–1.512863	–0.420612
6	–1.999024	–1.838024	–0.021760
1	–2.213628	–2.065823	–1.076839
1	–1.704970	–2.787088	0.433909
1	–2.945885	–1.512817	0.420834
6	–2.422951	1.300346	0.023265
1	–3.045365	0.935385	–0.797718
1	–2.946026	1.107092	0.964095
1	–2.281369	2.374539	–0.086679

NNCC5

SCF energy = –451.704784826

7	–1.147142	–1.021230	–0.003473
7	1.140609	–1.024188	–0.002025
6	–0.003994	–1.763088	–0.024711
5	–1.237582	0.425059	0.012989
7	–0.000827	1.139553	–0.023006
5	1.233096	0.420587	0.017843
6	2.366301	–1.825352	–0.007164
1	2.905358	–1.726174	0.939216
1	2.081464	–2.866027	–0.144466
1	3.031916	–1.521778	–0.818960
6	–2.372721	–1.823505	–0.009863
1	–3.023085	–1.543911	–0.842377
1	–2.083582	–2.866714	–0.114889
1	–2.928851	–1.700192	0.923466
6	–2.629415	1.174961	0.057363
1	–2.857418	1.626857	–0.916268
1	–3.473289	0.531503	0.308941
1	–2.622162	1.997391	0.779795
6	0.013238	2.599486	–0.065329
1	0.138808	3.031115	0.932918
1	0.829148	2.959876	–0.693140
1	–0.915807	2.984572	–0.483955
6	2.629713	1.159507	0.056152
1	3.433989	0.551729	0.474379
1	2.942396	1.428830	–0.961456
1	2.596319	2.093698	0.623475

NNPP5

SCF energy = –930.052501100

15	1.190306	–0.767669	–0.038511
6	–0.403550	–1.365679	0.144623
15	–1.538816	–0.411050	–0.788322
5	–0.508448	1.070329	–0.047331
5	1.134538	1.044222	–0.357804
6	2.528141	–1.829717	0.611364
1	2.821815	–2.577321	–0.126847
1	3.396781	–1.216845	0.858321
1	2.174737	–2.337792	1.508986
6	–3.132825	–0.571606	0.139073
1	–3.027827	–0.345556	1.200531
1	–3.880582	0.094624	–0.297817
1	–3.487100	–1.599196	0.035825
6	–1.161566	1.904779	1.124792
1	–1.104938	1.308583	2.045301
1	–0.635916	2.843159	1.323873
1	–2.221483	2.126531	0.968090
6	2.250011	2.124942	–0.550158
1	2.350536	2.327744	–1.624717
1	1.988608	3.080375	–0.085061
1	3.241294	1.827405	–0.196472

PHC

SCF energy = –1473.94325273

6	0.510447	–0.336503	1.585443
6	–0.114704	0.180937	–1.092416
15	1.107540	–0.529632	–0.138218
15	–1.246956	0.595960	0.103073
7	–0.718490	0.034599	1.652729
6	2.847597	–0.038556	–0.331793
6	3.223252	1.303144	–0.128433
6	3.802321	–1.021189	–0.646379
6	4.570244	1.637600	–0.243866
6	5.138236	–0.641975	–0.752897
6	5.519639	0.675525	–0.552430
1	4.875811	2.668182	–0.092435
1	5.886418	–1.388771	–0.999006
1	6.564601	0.954792	–0.640510
6	–2.987092	0.135240	–0.140081
6	–3.362928	–1.220337	–0.163226
6	–3.936129	1.156769	–0.311137
6	–4.706318	–1.531153	–0.354909
6	–5.268746	0.800444	–0.504648
6	–5.651669	–0.531413	–0.524660
1	–5.012190	–2.572622	–0.374781
1	–6.014129	1.577983	–0.639129
1	–6.694440	–0.791517	–0.675489
6	3.419359	–2.461693	–0.876486
6	2.213275	2.371792	0.192088
6	–2.354868	–2.324339	0.002766
6	–3.553348	2.615641	–0.296252
6	1.318885	–0.731629	2.781796
1	0.756028	–0.540306	3.695548
1	1.573370	–1.794787	2.739257
1	2.260725	–0.175533	2.812806
1	2.700122	3.337562	0.336556
1	1.652552	2.141561	1.103524
1	1.481333	2.473859	–0.612959
1	4.293733	–3.056645	–1.146190
1	2.975785	–2.909468	0.017507
1	2.685596	–2.558098	–1.680414
1	–1.833891	–2.242596	0.960289
1	–1.599248	–2.286263	–0.786744
1	–2.836326	–3.302665	–0.037297
1	–3.065689	2.893691	0.641842
1	–2.858890	2.856943	–1.105076
1	–4.435308	3.247750	–0.414101

Ph2CAuPMe3

SCF energy = –1097.70830059

79	–0.861824	–0.001892	0.002043
15	–3.194803	–0.001006	0.000185
6	–3.928865	–0.715961	1.498611
1	–5.019350	–0.689916	1.442008
1	–3.599950	–1.749902	1.613416
1	–3.602057	–0.153135	2.374354
6	–3.920381	–0.943874	–1.371876
1	–5.011084	–0.900495	–1.332547
1	–3.579402	–0.531807	–2.322850
1	–3.602365	–1.985956	–1.312713
6	–3.930352	1.653033	–0.138445
1	–5.020790	1.590067	–0.142423
1	–3.611802	2.271138	0.702461
1	–3.595369	2.127988	–1.061828
6	1.191681	0.000293	0.001044
6	1.922834	–1.238636	0.040073
6	1.357391	–2.413451	–0.505088
6	3.186338	–1.335010	0.668340
6	2.052450	–3.605210	–0.490584
1	0.381280	–2.363012	–0.975637
6	3.853111	–2.545171	0.727840
1	3.607590	–0.467126	1.160990
6	3.297496	–3.674109	0.133689
1	1.622956	–4.490377	–0.944691
1	4.805903	–2.613599	1.239485
1	3.827613	–4.619401	0.172473
6	1.918748	1.241687	–0.039322
6	1.349815	2.415269	0.504917
6	3.181426	1.341683	–0.668709
6	2.040591	3.609459	0.488092
1	0.374248	2.362206	0.976270
6	3.844000	2.554053	–0.730235
1	3.605244	0.474654	–1.160659
6	3.284924	3.681865	–0.137212
1	1.608341	4.493736	0.941318
1	4.796194	2.625081	–1.242639
1	3.811709	4.628941	–0.177742

aNHC

SCF energy = –1621.95414991

6	–0.344057	–1.906564	–0.676754
6	0.905583	–1.315541	–0.669067
6	–0.491753	0.316203	–0.101993

7	–1.163629	–0.828995	–0.324579
7	0.803525	0.037771	–0.298010
6	1.867507	0.930991	0.062798
6	2.170181	2.015257	–0.766616
6	2.554427	0.670271	1.256284
6	3.206598	2.856933	–0.368893
6	3.582303	1.541259	1.605913
6	3.907331	2.624152	0.803723
1	3.470503	3.708219	–0.988161
1	4.136035	1.370827	2.523447
1	4.711317	3.292063	1.095098
6	–1.080628	1.622147	0.220393
6	–2.144513	2.088834	–0.555569
6	–0.606781	2.413473	1.268268
6	–2.724302	3.319036	–0.288467
1	–2.510098	1.489848	–1.380595
6	–1.186958	3.647125	1.530412
1	0.222922	2.073173	1.874448
6	–2.246729	4.102600	0.755424
1	–3.547542	3.668402	–0.902002
1	–0.807459	4.253224	2.345804
1	–2.698481	5.066692	0.962909
6	–2.553199	–0.982990	–0.003235
6	–3.486752	–1.078629	–1.037378
6	–2.906907	–1.052303	1.349619
6	–4.823755	–1.246158	–0.684761
6	–4.256335	–1.215653	1.651763
6	–5.206099	–1.310255	0.646147
1	–5.578199	–1.328245	–1.459714
1	–4.571788	–1.280691	2.687391
1	–6.252724	–1.441261	0.901454
6	2.193208	–1.982555	–0.906477
6	3.331093	–1.334456	–1.394960
6	2.283314	–3.349875	–0.617614
6	4.527645	–2.021675	–1.558304
1	3.296606	–0.282036	–1.645063
6	3.474870	–4.035808	–0.791165
1	1.396846	–3.855974	–0.253218
6	4.608457	–3.373394	–1.252538
1	5.399193	–1.494234	–1.932612
1	3.522818	–5.094460	–0.556516
1	5.544302	–3.908002	–1.378279
6	–1.857467	–1.044064	2.450034
1	–0.956696	–0.563084	2.064387
6	1.425027	2.288471	–2.062251
1	0.632602	1.543665	–2.165827
6	2.348673	2.137972	–3.276486
1	1.792196	2.312611	–4.201569
1	3.170885	2.859126	–3.243787
1	2.781408	1.136569	–3.333586
6	0.764328	3.671847	–2.047097
1	0.146660	3.805690	–2.939574
1	0.126596	3.805385	–1.171377
1	1.513166	4.469700	–2.043496
6	2.212138	–0.499678	2.167777
1	1.427148	–1.093227	1.696038
6	3.416124	–1.427765	2.365112
1	3.119605	–2.308756	2.940964
1	3.816273	–1.771473	1.409483
1	4.222325	–0.930003	2.913361
6	1.665001	–0.015371	3.515454
1	1.403022	–0.870793	4.144889
1	2.400083	0.585119	4.059835
1	0.762058	0.588912	3.394640
6	–3.057161	–1.043267	–2.492677
1	–2.072221	–0.568413	–2.539012
6	–2.886874	–2.471330	–3.023737
1	–3.835744	–3.015787	–2.974875
1	–2.556356	–2.456304	–4.066973
1	–2.141705	–3.004959	–2.430570
6	–4.003798	–0.226282	–3.375996
1	–4.971208	–0.719433	–3.507219
1	–4.193035	0.768900	–2.961869
1	–3.570418	–0.101353	–4.371985
6	–2.277025	–0.246038	3.684121
1	–3.114673	–0.709146	4.213374
1	–1.444747	–0.190245	4.391643
1	–2.564898	0.774475	3.416757
6	–1.468488	–2.484697	2.801603
1	–2.323878	–3.030186	3.212615
1	–1.118957	–3.014193	1.911929
1	–0.668380	–2.495102	3.548693